

**David A Leigh, Publication List (6 April 2022)**

**2022**

303. 'Decorating beads with paramagnetic rings: synthesis of inorganic-organic  $[10^{14}]$ rotaxanes as shown by spin counting', D Asthana, D Thomas, S J Lockyer, A Brookfield, G A Timco, I J Vitorica-Yrezabal, G F S Whitehead, E J L McInnes, D Collison, D A Leigh and R E P Winpenny, *ChemRxiv*, Version 2, Feb 08, 2022.

302. 'Autonomous fuelled directional rotation about a covalent single bond', S Borsley, E Kreidt, D A Leigh and B M W Roberts, *Nature* **604**, 80-85 (2022).

301. 'Vernier template synthesis of molecular knots', Z Ashbridge, E Kreidt, L Pirvu, F Schaufelberger, J Halldin Stenlid, F Abild-Pedersen and D A Leigh, *Science*, **375**, 1035-1041 (2022).

[For highlights of this paper see, 'Chemists tie a knot with 12 crossings', *Chem & Eng News*, 11 March 2022; 'Химики получили циклический молекулярный узел с 12 перекрестьями' (in Russian), *NPlus1*, 3 March 2022; "错"就是对 : Science报道合成分子结的Vernier模板法" (in Chinese), K. Du, *X-Mol*, 11 March 2022; "把"分子打结"做到极致" (in Chinese), *Frontiers in Polymer Science*, 3 March 2022.]

300. 'Pumping between phases with a pulsed-fuel molecular ratchet', D Thomas, D J Tetlow, Y Ren, S Kassem, U Karaca and D A Leigh, *Nat Nanotechnol*, published online 4 April 2022.

299. 'Chemical fuels for molecular machinery', S Borsley, D A Leigh and B M W Roberts, *Nat Chem*, in press.

298. 'Molecular weaving', Z-H Zhang, B J Andreassen, D P August, D A Leigh and L Zhang, *Nat Mater*, **21**, 275-283 (2022).

[Featured on the cover of *Nat. Mater.*].

297. 'Insights from an information thermodynamics analysis of a synthetic molecular motor', S Amano, M Esposito, E Kreidt, D A Leigh, E Penocchio and B M W Roberts, *Nat Chem*, published online 17 March 2022.

**2021**

296. 'Real-time observation of the dynamics of an individual rotaxane molecular shuttle using a single molecule junction', S Chen, D Su, C Jia, Y Li, X Li, X Guo, D A Leigh and L Zhang, *Chem*, **8**, 243-252 (2022).

295. 'Chemical engines: Driving systems away from equilibrium through catalyst reaction cycles', S Amano, S Borsley, D A Leigh and Z Sun, *Nat Nanotechnol*, **16**, 1057-1067 (2021).

294. 'A catalysis-driven artificial molecular pump', S Amano, S D P Fielden and D A Leigh, *Nature*, **594**, 529-534 (2021).

293. 'Sequence-selective decapeptide synthesis by the parallel operation of two artificial molecular machines', J Echavarren, M A Y Gall, A Haertsch, D A Leigh, J T J Spence, D J Tetlow and C Tian, *J Am Chem Soc*, **143**, 5158-5165 (2021).

292. 'A doubly kinetically-gated information ratchet autonomously driven by carbodiimide hydration', S Borsley, D A Leigh and B M W Roberts, *J Am Chem Soc*, **143**, 4414-4420 (2021).

291. 'Site-to-site peptide transport on a molecular platform using a small-molecule robotic arm', S Kassem, A T L Lee, D A Leigh, A Markevicius, D J Tetlow and N Toriumi, *Chem Sci*, **12**, 2065-2070 (2021).

290. 'Effects of turn-structure on folding and entanglement in artificial molecular overhand knots', Y Song, F Schaufelberger, Z Ashbridge, L Pirvu, I J Vitorica-Yrezabal and D A Leigh, *Chem Sci*, **12**, 1826-1833 (2021).

289. 'Real-time fluctuations in single-molecule rotaxane experiments reveal an intermediate weak binding state during shuttling', D Sluysmans, P Lussis, C-A Fustin, A Bertocco, D A Leigh, A-S Duwez, *J Am Chem Soc*, **143**, 2348-2353 (2021).

288. 'A chiral cyclometalated Iridium Star of David [2]catenane', D P August, J Jaramillo-Garcia, D A Leigh, A Valero and I J Vitorica-Yrezabal, *J Am Chem Soc*, **143**, 1154-1161 (2021).

[For highlights of this paper see, 'Star of David catenane shines with both Ir and Zn', *Chem & Eng News*, **99**(2), (2021); 'Chiral star-shaped catenane', *ChemistryViews.Org*, 19 Jan 2021]

287. 'A molecular endless ( $7_4$ ) knot', D A Leigh, J J Danon, S D P Fielden, J-F Lemonnier, G F S Whitehead and S L Woltering, *Nat Chem*, **13**, 117-122 (2021).

[For highlights of this paper see, 'Untangling knotty problems' (N&Vs), D Preston and P E Kruger, *Nat Chem*, **13**, 114-116 (2021); 'Weaving on the molecular scale', Y Jiao and J F Stoddart, *Matter* **4**, 2582-2584 (2021); 'Chemists tie an 'endless' knot — one of the most complex ever made', *Nature*, 16 Dec 2020; '258-atom endless knot created with thiazole ligands', *Chem World*, 21 Dec 2020, etc]

**2020**

286. 'Self-assembly of a layered two-dimensional molecularly woven fabric', D P August, R A W Dryfe, S J Haigh, P R C Kent, D A Leigh, J-F Lemonnier, Z Li, C A Muryn, L I Palmer, Y Song, G F S Whitehead and R J Young, *Nature*, **588**, 429-435 (2020).

[For a highlight of this paper see, 'Weaving on the molecular scale', Y Jiao and J F Stoddart, *Matter* **4**, 2582-2584 (2021); 'Chemists weave molecular fabric', *Chem & Eng News*, **98**(48), (2020); 'Scientists awarded a Guinness World Record for the finest woven fabric', *Phys.Org*, 19 Jan 2021, etc]

285. 'Transmembrane ion channels formed by a Star of David [2]catenane and a molecular pentafoil knot', D P August, S Borsley, S L Cockroft, F della Sala, D A Leigh and S J Webb, *J Am Chem Soc*, **142**, 18859-18865 (2020).

284. 'A track-based molecular synthesizer that builds a single-sequence oligomer through iterative carbon-carbon bond formation', C McTernan, G De Bo and D A Leigh, *Chem*, **6**, 2964-2973 (2020). Featured on the cover of *Chem*.

[For highlights of this paper see, 'On the right "track" to artificial assemblers', R Costil, A Guinart and B L Feringa, *Chem*, **6**, 2868-2870 (2020); 'Diverging from nature: a new reactivity for molecular synthesizers', C T McTernan, *Chem*, **6**, 2862-2864 (2020); 'Editors' favorite articles 2020', *Chem*]

283. 'Tying different knots in a molecular strand', D P August, J Halldin Stenlid, D A Leigh, L Pirvu, F Schaufelberger and J Segard, *Nature*, **584**, 562-568 (2020).

[For highlights of this paper see, 'Tying knots in a molecular string', *Chem & Eng News*, **98**(34), (2020); 'Molecules of the Year 2020', *Chem & Eng News*, **98**(48), (2020), etc]

282. 'Knotted a molecular strand can invert macroscopic effects of chirality', N Katsonis, F Lancia, D A Leigh, L Pirvu, A Ryabchun and F Schaufelberger, *Nat Chem*, **12**, 939-944 (2020).

[For a highlight of this paper see, 'Knotted molecules can transfer chirality from the nano to the macroscale', *Chem World*, 6 Aug 2020]

281. 'Single-step enantioselective synthesis of mechanically planar chiral [2]rotaxanes using a chiral leaving group strategy', C Tian, S D P Fielden, B Pérez-Saavedra, I J Vitorica-Yrezabal, and D A Leigh, *J Am Chem Soc*, **142**, 9803-9808 (2020).

[For a highlight of this paper see, 'Point to mechanically chiral planes', T M Swager, B McDonald, *Synfacts*, **16**, 0917 (2020)]

280. 'Weak functional group interactions revealed through metal-free active template rotaxane synthesis', C Tian, S D P Fielden, G F S Whitehead, I J Vitorica-Yrezabal and D A Leigh, *Nat Commun*, **11**, 744 (2020).

[Featured in *Nat Commun Focus: Nanoscale & Supramolecular Chemistry*, 6 Feb 2020; for a highlight of this paper see: 'Party of Rotaxanes', T M Swager, Q He, *Synfacts*, **16**, 0405 (2020)]

## 2019

279. 'Dynamic control of chiral space through local symmetry breaking in a rotaxane organocatalyst', M Dommaschk, J Echavarren, D A Leigh, V Marcos and T A Singleton, *Angew Chem Int Ed*, **58**, 14955-14958 (2019).

278. 'Self-sorting assembly of molecular trefoil knots of single handedness', J Zhong, L Zhang, D August, G F S Whitehead and D A Leigh, *J Am Chem Soc*, **141**, 14249-14256 (2019).

277. 'Active template rotaxane synthesis through the Ni-catalyzed cross-coupling of alkylzinc reagents with redox-active esters', J Echavarren, M A Y Gall, A Haertsch, D A Leigh, V Marcos and D J Tetlow, *Chem Sci*, **10**, 7269-7273 (2019).

276. 'Dissipative catalysis with a molecular machine', C Biagini, S D P Fielden, D A Leigh, F Schaufelberger, S Di Stefano and D Thomas, *Angew Chem Int Ed*, **58**, 9876-9880 (2019).

[Hot Paper; featured on the cover of *Angew Chem Int Ed*].

275. 'Stereoselective synthesis of molecular square and granny knots', D A Leigh, L Pirvu and F Schaufelberger, *J Am Chem Soc*, **141**, 6054-6059 (2019).

274. 'Coordination chemistry of a molecular pentafoil knot', L Zhang, A J Stephens, J-F Lemonnier, L Pirvu, I J Vitorica-Yrezabal, C J Robinson and D A Leigh, *J Am Chem Soc*, **141**, 3952-3958 (2019).

273. 'Probing the dynamics of imine-based pentafoil knot and pentameric circular helicate assembly', J-F Ayme, J E Beves, C J Campbell and D A Leigh, *J Am Chem Soc*, **141**, 3605-3612 (2019).

272. 'Effects of knot tightness at the molecular level', L Zhang, J-F Lemonnier, A Acocella, M Calvaresi, F Zerbetto and D A Leigh, *Proc Natl Acad Sci USA*, **116**, 2452-2457 (2019).

[For a highlight of this paper see, 'Nano-nodi molecolari per i materiali del futuro (in Italian)', *Galileonet.it*, 31 Jan 2019]

## 2018

271. 'Analysis of two [2]catenanes based on electron densities from invariom refinement and results from DFT calculations', P Luger, B Dittrich, S Mebs, A M Z Slawin and D A Leigh, *Z. Naturforsch.*, **73b**, 677-687 (2018).

270. 'A six-crossing doubly interlocked [2]catenane with twisted rings, and a molecular granny knot', J J Danon, D A Leigh, S Pisano, A Valero and I J Vitorica-Yrezabal, *Angew Chem Int Ed*, **57**, 13833-13837 (2018).

[For a highlight of this paper see: 'Chemists weave granny and triple trefoil knots', *Chem World*, 11 Sept 2018]

269. 'Comment on "Coordination-Driven Self-Assembly of a Molecular Knot Comprising Sixteen Crossings"', D A Leigh, J-F Lemonnier and S L Woltering, *Angew Chem Int Ed*, **57**, 12212-12214 (2018).
268. 'Spontaneous assembly of rotaxanes from a primary amine, crown ether and electrophile', S D P Fielden, D A Leigh, C T McTernan, B Pérez-Saavedra and I J Vitorica-Yrezabal, *J Am Chem Soc*, **140**, 6049-6052 (2018).
267. 'Securing a supramolecular architecture by tying a stopper knot', D A Leigh, L Pirvu, F Schaufelberger, D J Tetlow and L Zhang, *Angew Chem Int Ed*, **57**, 10484-10488 (2018). [VIP paper]
266. 'Stereoselective synthesis of a composite knot with nine crossings' L Zhang, A J Stephens, A L Nussbaumer, J-F Lemonnier, P Jurček, I J Vitorica-Yrezabal and D A Leigh, *Nat Chem*, **10**, 1083-1088 (2018).  
[Featured on the cover of *Nature Chem*; for highlights of this paper see: 'What tangled webs we weave' (N&Vs), E E Fenlon, *Nat Chem*, 10 Sept 2018; 'Chemists tie most complex molecular knot to date', *Chem & Eng News*, 10 Sept 2018; 'The world's most complex molecular knot ties up a record', *Nature*, 10 Sept 2018; 'Chemists weave granny and triple trefoil knots', *Chem World*, 11 Sept 2018; 'Researchers create most tangled interlocked molecule ever', *Phys.org*, 12 Sept 2018; etc]
265. 'A molecular trefoil knot from a trimeric circular helicate' L Zhang, D P August, J Zhong, G F S Whitehead, I J Vitorica-Yrezabal and D A Leigh, *J Am Chem Soc*, **140**, 4982-4985 (2018).  
[For a highlight of this paper see: 'Molecular knot made from trimeric circular helicate', *ChemistryViews*, 22 March 2018]
264. 'An artificial molecular machine that builds an asymmetric catalyst' G De Bo, M A Y Gall, S Kuschel, J De Winter, P Gerbaux and D A Leigh, *Nat Nanotechnol*, **13**, 381-385 (2018).  
[For highlights of this paper see: "'Cyborg ribosome' decodes polystyrene message to manufacture catalyst', *Chem World*, 18 April 2018; 'Things molecules can do', *Nat Nanotech*, **13**, 353 (2018); etc]
263. 'Molecular machines with bio-inspired mechanisms' L Zhang, V Marcos and D A Leigh, *Proc Natl Acad Sci USA*, **115**, 9397-9404 (2018).
- 2017**
262. 'Transient two-dimensional vibrational spectroscopy of an operating molecular machine' M R Panman, C van Dijk, A Huerta-Viga, H J Sanders, B H Bakker, D A Leigh, A M Brouwer, W J Buma and S Woutersen, *Nat Commun*, **8**, 2206 (2017).
261. 'Enzyme-mediated directional transport of a small-molecule walker with chemically-identical feet' C J Martin, A T L Lee, R W Adams and D A Leigh, *J Am Chem Soc*, **139**, 11998-12002 (2017).
260. 'A complementary pair of enantioselective switchable organocatalysts' G De Bo, D A Leigh, C T McTernan, S Wang, *Chem Sci*, **8**, 7077-7081 (2017).
259. 'Rotary and linear molecular motors driven by pulses of a chemical fuel' S Erbas-Cakmak, S D P Fielden, U Karaca, D A Leigh, C T McTernan, D J Tetlow and M R Wilson, *Science*, **358**, 340-343 (2017).  
[For highlights of this paper see: 'Chemical fuel pulses power rotary and linear nanomotors', *Nanotechweb.org*, 26 Oct 2017; etc]
258. 'Sequence-specific beta-peptide synthesis by a rotaxane-based molecular machine' G De Bo, M A Y Gall, M O Kitching, S Kuschel, D A Leigh, D J Tetlow and J W Ward, *J Am Chem Soc*, **139**, 10875-10879 (2017).
257. 'Stereodivergent synthesis with a programmable molecular machine' S Kassem, A T L Lee, D A Leigh, V Marcos, L I Palmer and S Pisano, *Nature*, **549**, 374-378 (2017).  
[For highlights of this paper see: 'A molecular assembler' (N&Vs) T R Kelly and M L Snapper, *Nature*, **549**, 336-337 (2017); 'Molecular machine builds set of chiral molecules' (News-of-the-week) *Chem & Eng News*, **95**(38), 3 (2017); 'Single molecular machine produces four chiral products', *Chem World*, 21 Sep 2017; 'Research of the Year 2017', *Chem & Eng News*, 18 Dec 2017; 'Molecule-building and synthesis-planning machines', 2017s Biggest Chemistry Stories, *CompoundChem*, 30 Dec 2017; etc]
256. 'Switching between anion-binding catalysis and amino-catalysis with a rotaxane dual-function catalyst' K Eichstaedt, J Jaramillo-Garcia, D A Leigh, V Marcos, S Pisano and T A Singleton, *J Am Chem Soc*, **139**, 9376-9381 (2017).
255. '[2]Rotaxane formation by transition state stabilization' G De Bo, G Dolphijn, C T McTernan and D A Leigh, *J Am Chem Soc*, **139**, 8455-8457 (2017).
254. 'Molecular knots' S D P Fielden, D A Leigh and S L Woltering, *Angew Chem Int Ed*, **56**, 11166-11194 (2017).
253. 'Pyridyl-acyl hydrazone rotaxanes and molecular shuttles' D A Leigh, V Marcos, T Nalbantoglu, I J Vitorica-Yrezabal, F T Yasar and X Zhu, *J Am Chem Soc*, **139**, 7104-7109 (2017).  
[For a highlight of this paper see: 'Overcoming the limitations of molecular shuttles' *J Am Chem Soc*, **139**, 7131 (2017)]
252. 'Artificial molecular motors' S Kassem, T van Leeuwen, A S Lubbe, M R Wilson, B L Feringa and D A Leigh, *Chem Soc Rev*, **46**, 2592-2621 (2017).

251. 'Braiding a molecular knot with eight crossings' J J Danon, A Krüger, D A Leigh, J-F Lemonnier, A J Stephens, I J Vitorica-Yrezabal and S L Woltering, *Science*, **355**, 159-162 (2017).

[For highlights of this paper see: 'Tight embrace in a molecular knot with eight crossings', F B L Cougnon, *Angew Chem Int Ed*, **56**, 4918-4919 (2017); 'Braiding a molecular knot' (news-of-the-week) *Chem & Eng News*, **95**(3), 3 (2017); 'Braided molecules help scientists tie the knot', *Chem World*, 12 Jan 2017; 'Chemists have 'braided' molecules to make the tightest knot ever', *Forbes*, 13 Jan 2017; 'Knotty professors: chemists break world record to create tightest knot ever made', *The Guardian*, 12 Jan 2017; 'Molecules tied into beautiful 'octofoil' knot for first time', *New Scientist*, 12 Jan 2017; 'Molecular knot gets Guinness world record', *Chem World*, 21 Dec 2017; 'Molecules of the Year 2017', *Chem & Eng News*, 4 Dec 2017; 'Chemists break record for tightest ever knot', 2017s Biggest Chemistry Stories, *CompoundChem*, 30 Dec 2017; etc.]

## 2016

250. 'Genesis of the nanomachines: The 2016 Nobel Prize in Chemistry' D A Leigh, *Angew Chem Int Ed*, **55**, 14506-14508 (2016).

249. 'Tying a molecular overhand knot of single handedness and asymmetric catalysis with the corresponding pseudo-D3-symmetric trefoil knot' G Gil-Ramírez, S Hoekman, M O Kitching, D A Leigh, I Vitorica-Yrezabal and G Zhang, *J Am Chem Soc*, **138**, 13159-13162 (2016).

[For a highlight of this paper see: 'Chiral complexes tie the knot' *Chem World*, 6 Oct 2016]

248. 'Triply-threaded [4]rotaxanes' J J Danon, D A Leigh, P R McGonigal, J W Ward and J Wu, *J Am Chem Soc*, **138**, 12643-12674 (2016).

[For a highlight of this paper see: 'Chemists cultivate 'macromolecular wheatsheaf'' *Chem World*, 20 Sept 2016]

247. 'Successive translocation of the rings in a [3]rotaxane' D C Jagesar, P G Wiering, E R Kay, D A Leigh and A M Brouwer, *ChemPhysChem*, **17**, 1902-1912 (2016).

246. 'Allosteric initiation and regulation of catalysis with a molecular knot' V Marcos, A J Stephens, J Jaramillo-Garcia, A L Nussbaumer, S L Woltering, A Valero, J-F Lemonnier, I J Vitorica-Yrezabal and D A Leigh, *Science*, **352**, 1555-1559 (2016).

[For highlights of this paper see: 'Molecular knot ties up anions to catalyse reactions' *Chem & Eng News*, **94**(26), 8 (2016); 'Molecular knot inducing allosteric control of catalysis' T M Swager and C-C A Voll, *Synfacts*, **12**, 911 (2016); etc.]

245. 'An autonomous chemically fuelled small-molecule motor' M R Wilson, J Solà, A Carlone, S M Goldup, N Lebrasseur and D A Leigh, *Nature*, **534**, 235-240 (2016).

[For highlights of this paper see: 'No turning back for motorized molecules' (N&Vs), J Clayden, *Nature*, **34**, 187-188 (2016); 'Artificial molecular motors: Running on information' (N&Vs), R D Astumian, *Nat Nanotech*, **11**, 582-583 (2016); 'Autonomous chemically fueled molecular motor revs up' (news-of-the-week), *Chem & Eng News*, **94**(24), 4 (2016); 'Molecular motors start chemically-fuelled journey' *Chem World*, 9 June 2016; 'Chemical Highlights of 2016' *Chem World*, 15 Dec 2016, etc.]

244. 'Asymmetric catalysis with a mechanically point-chiral rotaxane' Y Cakmak, S Erbas-Cakmak and D A Leigh, *J Am Chem Soc*, **138**, 1749-1751 (2016).

[For highlights of this paper see: 'A chiral catalyst with a ring to it' (N&Vs) S M Goldup, *Nat Chem*, **8**, 404-406 (2016); 'Rare new form of chirality observed in rotaxanes', *JACS Spotlight*, *J Am Chem Soc*, **138**, 2063 (2016)]

243. 'Making the tiniest machines' D A Leigh in 'Macrocyclic and Supramolecular Chemistry: How Izatt-Christensen Award Winners Shaped the Field' R Izatt (ed.), Wiley, p. 241-260 (2016).

242. 'Pick-up, transport and release of a molecular cargo using a small-molecule robotic arm' S Kassem, A T L Lee, D A Leigh, A Markevicius and J Solà, *Nat Chem*, **8**, 138-143 (2016).

[For highlights of this paper see: 'Molecules bearing robotic arms' (N&Vs), I Aprahamian, *Nat Chem*, **8**, 97-99 (2016); 'Molecular robot opens the way to nano-assembly lines', *Chem World*, 5 Jan 2016; 'Chemical Highlights of 2016' *Chem World*, 15 Dec 2016, etc.]

## 2015

241. 'Artificial molecular machines' S Erbas-Cakmak, D A Leigh, C T McTernan and A L Nussbaumer, *Chem Rev*, **115**, 10081-10206 (2015).

240. 'Lanthanide template synthesis of trefoil knots of single handedness' G Zhang, G Gil-Ramírez, A Markevicius, C Browne, I J Vitorica-Yrezabal and D A Leigh, *J Am Chem Soc*, **137**, 10437-10442 (2015).

239. 'Strong and selective anion binding within the central cavity of molecular knots and links' J-F Ayme, J E Beves, C J Campbell, G Gil-Ramírez, D A Leigh and A J Stephens, *J Am Chem Soc*, **137**, 9812-9815 (2015).

[Featured on the cover of *J Am Chem Soc*. For a highlight of this paper see: 'Ready or knot, here come synthetic anion-binding molecules', *JACS Spotlight*, *J Am Chem Soc*, **137**, 9759 (2015).]

238. 'Goldberg active template synthesis of a [2]rotaxane ligand for asymmetric transition metal catalysis' S Hoekman, M O Kitching, D A Leigh, M Papmeyer and D Roke, *J Am Chem Soc*, **137**, 7656-7659 (2015).  
[For a highlight of this paper see: 'Enantioselective Michael addition using a Nickel/rotaxane catalyst', M Lautens, Z Qureshi, *Synfacts*, **11**, 0839 (2015)]
237. 'Rise of the molecular machines' E R Kay and D A Leigh, *Angew Chem Int Ed*, **54**, 10080-10088 (2015).
236. 'Artificial switchable catalysts' V Blanco, D A Leigh, and V Marcos, *Chem Soc Rev*, **44**, 5341-5370 (2015).
235. 'A Solomon Link through an interwoven molecular grid' J E Beves, J J Danon, D A Leigh, J-F Lemonnier and I J Vitorica-Yrezabal, *Angew Chem Int Ed*, **54**, 7555-7559 (2015). [Featured on the cover of *Angew Chem Int Ed*].
234. 'Catenanes: Fifty years of molecular links' G Gil-Ramírez, D A Leigh and A J Stephens, *Angew Chem Int Ed*, **54**, 6110-6150 (2015).
233. 'A mechanically interlocked molecular system programmed for the delivery of an anticancer drug' R Barat, T Legigan, I Tranoy-Opalinski, B Renoux, E Péraudeau, J Clarhaut, P Poinot, A E Fernandes, V Aucagne, D A Leigh and S Papot, *Chem Sci*, **6**, 2608-2613 (2015).
232. 'Selecting reactions and reactants using a switchable rotaxane organocatalyst with two different active sites' J Beswick, V Blanco, G De Bo, D A Leigh, U Lewandowska, B Lewandowski and K Mishiro, *Chem Sci*, **6**, 140-143 (2015).  
[For highlights of this paper see: 'One rotaxane, two catalytic stories' *Chem World*, 3 Dec 2014; 'Switching activation modes in an organocatalyst' *Chem Sci Blog*, 19 Nov 2014.]
231. 'A rotaxane-like supramolecular assembly featuring orthogonal recognition modes' D Menozzi, D A Leigh and E Dalcanale, *Asian J Org Chem*, **4**, 204-207 (2015).
- 2014**
230. 'Exploring the activation modes of a rotaxane-based switchable organocatalyst' V Blanco, D A Leigh, U Lewandowska, B Lewandowski and V Marcos, *J Am Chem Soc*, **136**, 15775-15780 (2014).  
[For a highlight of this paper see: 'The multiple lives of a switchable catalyst' *JACS Spotlight*, *J Am Chem Soc*, **136**, 15109-15110 (2014).]
229. 'Rotaxane catalysts' D A Leigh, V Marcos and M R Wilson, *ACS Catalysis*, **4**, 4490-4497 (2014).
228. 'A simple and highly effective ligand system for the copper(I)-mediated assembly of rotaxanes' C J Campbell, D A Leigh, I J Vitorica-Yrezabal and S L Woltering, *Angew Chem Int Ed*, **53**, 13771-13774 (2014).
227. 'Lanthanide template synthesis of a molecular trefoil knot' J-F Ayme, G Gil-Ramírez, D A Leigh, J-F Lemonnier, A Markevicius, C A Muryn and G Zhang, *J Am Chem Soc*, **136**, 13142-13145 (2014).
226. 'The self-sorting behavior of circular helicates and molecular knots and links' J-F Ayme, J E Beves, C J Campbell, and D A Leigh, *Angew Chem Int Ed*, **53**, 7823-7827 (2014).
225. 'A Star of David catenane' D A Leigh, R G Pritchard and A J Stephens, *Nat Chem*, **6**, 978-982 (2014).  
[For highlights of this paper see: 'Molecular topology: Star-crossed self-assembly (N&Vs)' G H Clever, *Nat Chem*, **6**, 950-952 (2014); 'Molecular knot shaped like a Star of David' *Chem World*, published online 22 Sept 2014; 'Star of David recreated as a molecular knot' *Sci Am*, 24 Sept 2014; 'Scientists create a 'Star of David' molecule—a step towards molecular chainmail' *Washington Post*, 22 Sept 2014; 'Generating a molecule with star quality' *NY Times*, 29 Sept 2014; 'New 'star' shaped molecule breakthrough' *Phys Org*, 22 Sept 2014; etc]
224. 'Synthetic molecular walkers' D A Leigh, U Lewandowska, B Lewandowski and M R Wilson, *Top Curr Chem*, **354**, 111-138 (2014).
223. 'Efficient assembly of threaded molecular machines for sequence-specific synthesis' G De Bo, S Kuschel, D A Leigh, B Lewandowski, M Papmeyer and J W Ward, *J Am Chem Soc*, **136**, 5811-5814 (2014).  
[For a highlight of this paper see: 'A more efficient way to thread a molecular machine' *JACS Spotlights*, *J Am Chem Soc* **136**, 5820 (2014)]
222. 'A switchable [2]rotaxane asymmetric organocatalyst that utilizes an acyclic chiral secondary amine' V Blanco, D A Leigh, V Marcos, J A Morales-Serna and A L Nussbaumer, *J Am Chem Soc*, **136**, 4905-4908 (2014).  
[For a highlight of this paper see: 'Ring around the catalyst' *Chem & Eng News*, **92**(14), 35 (2014)]
221. 'Probing the mobility of catenane rings in single molecules' D A Leigh, A-S Duwez, P Lussis, C-A Fustin and A Van Quaethem, *Chem Sci*, **5**, 1449-1452 (2014).  
[For a highlight of this paper see 'A catenane in action' *Nat Nanotech*, **9**, 161 (2014)]
220. 'Towards metal complexes that can directionally walk along tracks: Controlled stepping of a molecular biped with a Palladium(II) foot' J E Beves, V Blanco, B A Blight, R Carrillo, D M D'Souza, D C Howgego, D A Leigh, A M Z Slawin and M D Symes, *J Am Chem Soc*, **136**, 2094-2100 (2014).  
[For a highlight of this paper see: 'Molecular walker' *Chem & Ind*, **78**, 52 (2014)]

**2013**

219. 'Water lubricates hydrogen-bonded molecular machines' M R Panman, B H Bakker, D den Uyl, E R Kay, D A Leigh, W J Buma, A M Brouwer, J A J Geenevasen and S Woutersen, *Nat Chem*, **5**, 929-934 (2013).

[For highlights of this paper see: 'Water lubricates molecular machines' *Chem & Eng News*, **91**(35), 43 (2013); 'Water acts as a lubricant for molecular machines' *Chem World*, 1 Sept 2013]

218. 'AAAA-DDDD quadruple hydrogen bond arrays featuring NH $\cdots$ N and CH $\cdots$ N hydrogen bonds' D A Leigh, C C Robertson, A M Z Slawin and P I T Thomson, *J Am Chem Soc*, **135**, 9939-9943 (2013).

217. 'Tetrameric cyclic double helicates as a scaffold for a molecular Solomon Link' J E Beves, C J Campbell, D A Leigh, and R G Pritchard, *Angew Chem Int Ed*, **52**, 6464-6467 (2013). ['VIP' paper; featured on the cover]

216. 'The one dimensional random walk of a synthetic small molecule toward a thermodynamic sink' A G Campaña, D A Leigh and U Lewandowska, *J Am Chem Soc*, **135**, 8639-8645 (2013).

215. 'Induction of motion in a synthetic molecular machine: effect of tuning the driving force' J Baggerman, N Haraszkiwicz, P G Wiering, G Fioravanti, M Marcaccio, F Paolucci, E R Kay, D A Leigh and A M Brouwer, *Chem Eur J*, **19**, 5566-5577 (2013).

214. 'Sequence-specific peptide synthesis by an artificial small-molecule machine' B Lewandowski, G De Bo, J W Ward, M Pappmeyer, S Kuschel, M J Aldegunde, P M E Gramlich, D Heckmann, S M Goldup, D M D'Souza, A E Fernandes and D A Leigh, *Science*, **339**, 189-193 (2013).

[For highlights of this paper see: 'Interlocked molecules: A molecular production line (N&Vs)' P R McGonigal, J F Stoddart, *Nat Chem*, **5**, 260-262 (2013); 'A supramolecular peptide synthesizer' J Bertran-Vicente, C P R Hackenberger, *Angew Chem Int Ed*, **52**, 6140-6142 (2013); 'Molecular robot mimics life's protein-builder' *Nature*, **493**, 274 (2013); 'Robot ribosome (News-of-the-Week)' *Chem & Eng News*, **91**(2), 5 (2013); 'Peptide pick up' *Nature Nanotech*, **8**, 75 (2013); 'Chemistry riffs on the ribosome (Spotlight)' J G Underwood, *ACS Chem Biol*, **8**, 273-273 (2013); 'Synthesis of a peptide with an artificial molecular machine' T M Swager, D K Frantz, *SynFacts*, **9**, 273 (2013); 'Rotaxane mimics ribosome to spin out peptides' *Chem World*, 10 Jan 2013; 'Nanomachine mimics nature's protein factory' *New Scientist*, 10 Jan 2013; 'Tiny molecular machine apes cellular production line' *BBC News*, 11 Jan 2013; 'Ribosome robot' in *Breakthroughs of the Year 2013*, *Science* **342**, 1441 (2013); 'Top Chemistry Moments of 2013', *C&EN Webinar*, 10 Jan 2014; etc]

213. 'Template synthesis of molecular knots' J-F Ayme, J E Beves, C J Campbell and D A Leigh, *Chem Soc Rev*, **42**, 1700-1712 (2013). [Featured on the cover].

**2012**

212. 'A scalable synthesis of 5,5'-dibromo-2,2'-bipyridine and its stepwise functionalization via Stille couplings' D M D'Souza, D A Leigh, M Pappmeyer and S L Woltering, *Nat Protocols*, **7**, 2022-2028 (2012).

211. 'Pentameric circular iron(II) double helicates and a molecular pentafoil knot' J-F Ayme, J E Beves, D A Leigh, R T McBurney, K Rissanen and D Schultz, *J Am Chem Soc*, **134**, 9488-9497 (2012).

210. 'Half-rotation in a kinetically locked [2]catenane induced by transition metal ion substitution' D A Leigh, P J Lusby, A M Z Slawin and D B Walker, *Chem Commun*, **48**, 5826-5828 (2012).

209. 'A three-compartment chemically-driven molecular information ratchet' A Carlone, S M Goldup, N Lebrasseur, D A Leigh and A Wilson, *J Am Chem Soc*, **134**, 8321-8323 (2012).

[For a highlight of this paper see: 'Ratcheting up to a molecular motor' *JACS Spotlights*, June 2012]

208. 'A small molecule that walks non-directionally along a track without external intervention' A G Campaña, A Carlone, K Chen, D T F Dryden, D A Leigh, U Lewandowska and K M Mullen, *Angew Chem Int Ed*, **51**, 5480-5483 (2012).

[Featured on the cover. For highlights of this paper see: 'On the right track' *Nat Chem*, **4**, 430-431 (2012); 'Walk on by: The light at the end of the track' D Bradley, *SpectroscopyNow*, 15 May 2012; 'A Two-Legged Molecule' *Angew Chem Int Ed* press report, 24 April 2012]

207. 'A rotaxane-based switchable organocatalyst' V Blanco, A Carlone, K D Hänni, D A Leigh and B Lewandowski, *Angew Chem Int Ed*, **51**, 5166-5169 (2012).

[For highlights of this paper see: 'Switchable catalysis' U Lüning, *Angew Chem Int Ed*, **51**, 8163-8165 (2012), 'Controlling an organocatalyst with pH' *Chem World*, 19 April 2012]

206. 'Second generation specific-enzyme-activated rotaxane propeptides' A Fernandes, A Viterisi, V Aucagne, D A Leigh and S Papot, *Chem Commun*, **48**, 2083-2085 (2012). [Selected as a *Chem Commun* 'Hot Article' 2012]

205. 'A synthetic molecular pentafoil knot' J-F Ayme, J E Beves, D A Leigh, R T McBurney, K Rissanen and D Schultz, *Nat Chem*, **4**, 15-20 (2012). [Featured on the front cover]

[For highlights of this paper see: 'One-pot pentaknot (N&Vs)' M J Hardie, *Nat Chem*, **4**, 7-8 (2012); 'Molecule tied in pentafoil knot' *Chem & Eng News*, **89**(45), 25 (2011); 'Single molecule ties its way into famous knot' *New Scientist*, 7 Nov 2011; 'Edinburgh atom-weaving could strengthen plastic' *BBC News*, 7 Nov 2011; 'Scots team weaves way to stronger

plastics' *The Scotsman*, 7 Nov 2011; 'New technique holds promise for lighter, stronger plastics' *Eureka magazine*, 7 Nov 2011; 'Chemists create world's most complex molecular knot' *R&D magazine*, 7 Nov 2011; 'Scientists hail atom-weaving breakthrough' *World News Australia*, 7 Nov 2011; 'Chemical Highlights of 2011', *Chem World*, 20 Dec 2011; 'Image of the Year 2011' *Diamond Light Source*, 21 Dec 2011; 'Top-10 Nature Chemistry downloads of 2012' *thescepticalchymist*, 28 Dec 2012 etc]

204. 'Time-resolved vibrational spectroscopy of a molecular shuttle' M R Panman, P Bodis, D J Shaw, B H Bakker, A C Newton, E R Kay, D A Leigh, W J Buma, A M Brouwer and S Woutersen, *Phys Chem Chem Phys*, **14**, 1865-1875 (2012). [Featured on the cover.]

## 2011

203. 'Active metal template synthesis of a molecular trefoil knot' P E Barran, H L Cole, S M Goldup, D A Leigh, P R McGonigal, M D Symes, J Wu and M Zengerle, *Angew Chem Int Ed*, **50**, 12280-12284 (2011).

[Featured on the cover. For highlights of this paper see: 'Combining coordination chemistry and catalysis to tie a knot by an active-metal template strategy' C Romuald and F Coutrot, *Angew Chem Int Ed*, **51**, 2544-2545 (2012)]

202. 'Strategies and tactics for the metal-directed synthesis of rotaxanes, knots, catenanes and higher order links' J E Beves, B A Blight, C J Campbell, D A Leigh and R T McBurney, *Angew Chem Int Ed*, **50**, 9260-9327 (2011).

201. 'A single synthetic small molecule that generates force against a load' P Lussis, T Svaldo-Lanero, A Bertocco, C-A Fustin, D A Leigh and A-S Duwez, *Nat Nanotech*, **6**, 553-557 (2011).

[For highlights of this paper see: 'Manmade molecular machine goes to work' *Chem World*, 22 Aug 2011; 'Measuring the force of a single synthetic small molecule' *Nanowerk*, 26 Aug 2011; etc]

200. 'Phosphorus-based functional groups as hydrogen bonding templates for rotaxane formation' R Ahmed, A Altieri, D M D'Souza, D A Leigh, K M Mullen, M Papmeyer, A M Z Slawin, J K Y Wong and J D Woollins, *J Am Chem Soc*, **133**, 12304-12310 (2011).

199. 'En route to a molecular sheaf: Active metal template synthesis of a [3]rotaxane with two axles threaded through one ring' H M Cheng, D A Leigh, F Maffei, P R McGonigal, A M Z Slawin and J Wu, *J Am Chem Soc*, **133**, 12298-12303 (2011).

198. 'Sulfur-containing amide-based [2]rotaxanes and molecular shuttles' A Altieri, V Aucagne, R Carrillo, G J Clarkson, D M D'Souza, J A Dunnett, D A Leigh and K M Mullen, *Chem Sci*, **2**, 1922-1928 (2011).

197. 'IR spectroscopy on jet-cooled isolated two-station rotaxanes' A M Rijs, E R Kay, D A Leigh and W J Buma, *J Phys Chem A*, **115**, 9669-9675 (2011).

196. 'Walking molecules' M von Delius and D A Leigh, *Chem Soc Rev*, **40**, 3656-3676 (2011).

[For a highlight of this paper, see: 'Synthetic Strollers' S Everts, *Chem & Eng News*, **89**(12), 43-45 (2011); 'Walking in the nanoworld' M Gross, *Chem Ind*, 10 Oct 2011; Top 10 most highly accessed *Chem Soc Rev* article March 2011]

195. 'Bimodal dynamics of mechanically constrained hydrogen bonds revealed by vibrational photon echoes' P Bodis, S Yeremenko, J Berná, W J Buma, D A Leigh and S Woutersen, *J Chem Phys*, **134**, 134504 (2011).

194. 'An AAAA-DDDD quadruple hydrogen bond array' B A Blight, C A Hunter, D A Leigh, H McNab and P I T Thomson, *Nat Chem*, **3**, 244-248 (2011).

[For a highlight of this paper see: 'Attractive Arrays', A J Wilson, *Nat Chem*, **3**, 193-194 (2011)].

193. 'Light-driven transport of a molecular walker in either direction along a molecular track' M J Barrell, A G Campaña, M von Delius, E M Geertsema and D A Leigh, *Angew Chem Int Ed*, **50**, 285-290 (2011).

[Featured on the front cover of 50<sup>th</sup> Anniversary Issue; for highlights see: For highlights of this paper see: 'Synthetic Molecular Bipeds', E M Pérez, *Angew Chem Int Ed*, **50**, 3359-3361 (2011); 'Walking molecule follows the light', *Chem & Eng News*, **88**(43), 44 (2010)]

## 2010

192. 'Design, synthesis and operation of small molecules that walk along tracks' M von Delius, E M Geertsema, D A Leigh and D-T D Tang, *J Am Chem Soc*, **132**, 16134-16145 (2010).

191. 'Synthesis, structure and dynamic properties of hybrid organic-inorganic rotaxanes' B Ballesteros, T B Faust, C-F Lee, D A Leigh, C A Muryn, R G Pritchard, D Schultz, S J Teat, G A Timco and R E P Winpenny, *J Am Chem Soc*, **132**, 15435-15444 (2010).

190. 'Synthesis and solid state structure of a hydrazone-disulfide macrocycle and its dynamic covalent ring-opening under acidic and basic conditions' M von Delius, E M Geertsema, D A Leigh and A M Z Slawin, *Org Biomol Chem*, **8**, 4617-4624 (2010). [Selected as an OBC "Hot Article" 2010]

189. 'Linking rings without templates (N&Vs)' J E Beves and D A Leigh, *Nat Chem*, **2**, 708-710 (2010).

188. 'Ligand-assisted nickel-catalysed  $sp^3$ - $sp^3$  homocoupling of unactivated alkyl bromides and its application to the active template synthesis of rotaxanes' S M Goldup, D A Leigh, R T McBurney, P R McGonigal and A Plant, *Chem Sci*, **1**, 383-386 (2010).

187. 'Nitron [2]rotaxanes: Simultaneous chemical protection and electrochemical activation of a functional group' D M D'Souza, D A Leigh, L Mottier, K M Mullen, F Paolucci, S J Teat and S Zhang, *J Am Chem Soc*, **132**, 9465-9470 (2010).

186. 'Operation mechanism of a molecular machine revealed using time-resolved vibrational spectroscopy' M R Panman, P Bodis, D J Shaw, B H Bakker, A C Newton, E R Kay, A M Brouwer, W J Buma, D A Leigh and S Woutersen, *Science*, **328**, 1255-1258 (2010).

[For highlights of this paper see 'Molecular machine's movement turns out to be a dishonest gambling game' *FOM*, 4 June 2010; 'Motion of molecular machinery appears unfair' *AllePersberichten* (in Dutch), 4 June 2010]

185. 'In trap fragmentation and optical characterization of rotaxanes' A M Rijs, I Compagnon, A Silva, J S Hannam, D A Leigh, E R Kay and P Dugourd, *Phys Chem Chem Phys*, **12**, 12556-12561 (2010).

184. 'Controlled hydrogen-bond breaking in a rotaxane by discrete solvation: Stepwise release of a molecular brake' A M Rijs, N Saendig, M Blom, J Oomens, J S Hannam, D A Leigh, F Zerbetto and W J Buma, *Angew Chem Int Ed*, **49**, 3896-3900 (2010).

183. 'An unusual nickel-copper-mediated alkyne homocoupling reaction for the active template synthesis of [2]rotaxanes' J D Crowley, S M Goldup, N D Gowans, D A Leigh, V E Ronaldson and A M Z Slawin, *J Am Chem Soc*, **132**, 6243-6248 (2010).

182. 'Diels-Alder active template synthesis of rotaxanes and metal-ion-switchable molecular shuttles' J D Crowley, K D Hänni, D A Leigh and A M Z Slawin, *J Am Chem Soc*, **132**, 5309-5314 (2010).

181. 'Sequence isomerism in [3]rotaxanes' A-M L Fuller, D A Leigh and P J Lusby, *J Am Chem Soc*, **132**, 4954-4959 (2010).

180. 'Improved dynamics and positional bias with a second generation palladium(II)-complexed molecular shuttle' D A Leigh, P J Lusby, R T McBurney and M D Symes, *Chem Commun*, **46**, 2382-2384 (2010).

179. 'A synthetic small molecule that can walk down a track' M von Delius, E M Geertsema and D A Leigh, *Nat Chem*, **2**, 96-101 (2010).

[Featured on the front cover; for highlights of this paper see: 'Tiny Steps (N&Vs)' S Otto, *Nat Chem*, **2**, 75-76 (2010); 'Big Steps for Little Feet' *Science*, **327**, 127 (2010); "'Two-legged' molecular walker takes a stroll' *Chem World*, 21 Dec 2009; 'Tiny molecular track walker' *Chem & Eng News*, **87**(51), 34 (2009); 'Tiny molecules walk the track' *Science News*, 12 Feb 2010; 'Edinburgh motive force for NEMS' *Compute Scotland*, 21 Dec 2009; 'Chemical Highlights of 2010', *Chem World*, 21 Dec 2010; etc]

178. 'The application of CuAAC 'click' chemistry to catenane and rotaxane synthesis' K D Hänni and D A Leigh, *Chem Soc Rev*, **39**, 1240-1251 (2010).

[Top 10 most-downloaded *Chem Soc Rev* article April 2010]

177. 'Two axles threaded using a single template site: Active metal template macrobicyclic [3]rotaxanes' S M Goldup, D A Leigh, P R McGonigal, V E Ronaldson and A M Z Slawin, *J Am Chem Soc*, **132**, 315-320 (2010).

[For a highlight of this paper see 'Templated Threading to [3]Rotaxanes' T M Swager and B Esser, *Synfacts*, 301 (2010)]

## 2009

176. 'Photoinduced shuttling dynamics of rotaxanes in viscous polymer solutions' D C Jagesar, S M Fazio, J Taybi, E Eiser, F G Gatti, D A Leigh and A M Brouwer, *Adv Funct Mater*, **19**, 3440-3449 (2009).

175. 'Active metal template synthesis of [2]catenanes' S M Goldup, D A Leigh, T Long, P R McGonigal, M D Symes and J Wu, *J Am Chem Soc*, **131**, 15924-15929 (2009).

174. 'AAA-DDD Triple hydrogen bond complexes' B Blight, A Camara-Campos, S Djurdjevic, M Kaller, D A Leigh, F McMillan, H McNab and A M Z Slawin, *J Am Chem Soc*, **131**, 14116-14122 (2009).

173. 'Two-dimensional vibrational spectroscopy of rotaxane-based molecular machines' P Bodis, M R Panman, B H Bakker, A Mateo-Alonso, M Prato, W J Buma, A M Brouwer, E R Kay, D A Leigh and S Woutersen, *Acc Chem Res*, **42**, 1462-1469 (2009).

172. 'Conformational flexibility of a rotaxane thread probed by electronic spectroscopy in helium nanodroplets' S. Smolarek, A M Rijs, J S Hannam, D A Leigh, M Drabbels and W J Buma, *J Am Chem Soc*, **131**, 12902-12903 (2009).

171. 'Rotaxane-based propeptides: Protection and enzymatic release of a bioactive pentapeptide' A Fernandes, A Viterisi, F Coutrot, S Potok, D A Leigh, V Aucagne and S Papot, *Angew Chem Int Ed*, **48**, 6443-6447 (2009). ['Hot' paper].

170. 'Active metal template synthesis of rotaxanes, catenanes and molecular shuttles' J D Crowley, S M Goldup, A-L Lee, D A Leigh and R T McBurney, *Chem. Soc. Rev.*, **38**, 1530-1541 (2009).



169. 'Hybrid organic-inorganic rotaxanes and molecular shuttles' C-F Lee, D A Leigh, R G Pritchard, D Schultz, S J Teat, G A Timco and R E P Winpenny, *Nature*, **458**, 314-318 (2009).

[For highlights of this paper see: 'The marriage of inorganic and organic building blocks for the assembly of rotaxanes' E. K. Brechin, L. Cronin, *Angew. Chem. Int. Ed.*, **48**, 6948-6949 (2009); 'Rotaxanes go hybrid' *Chem & Eng News*, **87**(12), 11 (2009); 'Major leap for faster computers' BBC News, 19 March 2009; 'Scientists make quantum leap in developing faster computers' *Nanotechnology Now*, 20 March 2009 etc]

168. 'Getting harder: Cobalt(III)-template synthesis of catenanes and rotaxanes' D A Leigh, P J Lusby, R T McBurney, A Morelli, A M Z Slawin, A R Thomson and D B Walker, *J Am Chem Soc*, **131**, 3762-3771 (2009).

167. 'Stiff and sticky at the right places: Binding interactions in isolated mechanically interlocked molecules probed by mid-infrared spectroscopy' A M Rijs, I Compagnon, J Oomens, J S Hannam, D A Leigh and W J Buma, *J Am Chem Soc*, **131**, 2428-2429 (2009).

166. 'Multistate photo-induced relaxation and photoisomerization ability of fumaramide threads: a computational and experimental study' P Altoè, N Haraszkiwicz, F G Gatti, P G Wiering, C Frochot, A M Brouwer, G Balkowski, D Shaw, S Woutersen, W J Buma, F Zerbetto, G Orlandi, D A Leigh and M Garavelli, *J Am Chem Soc*, **131**, 104-117 (2009).

## 2008

165. 'A novel ion pair template for rotaxane formation and its exploitation in an orthogonal interaction anion switchable molecular shuttle' M J Barrell, D A Leigh, P J Lusby and A M Z Slawin, *Angew Chem Int Ed*, **47**, 8036-8039 (2008).

164. 'Core level photoemission of rotaxanes: a summary of binding energies' S M Mendoza, J Berná, E M Pérez, E R Kay, A Mateo-Alonso, C De Nadaï, S Zhang, J Baggerman, P G Wiering, D A Leigh, M Prato, A M Brouwer and P Rudolf, *J Electron Spec Rel Phenom*, **165**, 42-45 (2008).

163. 'Gold(I) template catenane and rotaxane synthesis' S M Goldup, D A Leigh, P J Lusby, R T McBurney and A M Z Slawin, *Angew Chem Int Ed*, **47**, 6999-7003 (2008).

[Featured on the front cover, issue 37, Sept 2008; for a highlight of this paper see 'Molecule-of-the-Week' *notjustanotherchemblog*, 30 August, 2008]

162. 'An ammonium/bis-ammonium switchable molecular shuttle' D A Leigh and A R Thomson, *Tetrahedron*, **64**, 8411-8416 (2008).

161. 'Cadiot-Chodkiewicz active template synthesis of rotaxanes and switchable molecular shuttles with weak intercomponent interactions' J Berná, S M Goldup, A-L Lee, D A Leigh, M D Symes, G Teobaldi and F Zerbetto, *Angew Chem Int Ed*, **47**, 4392-4396 (2008).

160. 'Tuning magnetic properties using targeted structural distortion: New additions to a family of Mn<sub>6</sub> single-molecule magnets' L F Jones, M E Cochrane, B D Koivisto, D A Leigh, S P Perlepes, W Wernsdorfer, E K Brechin, *Inorg Chim Acta*, **361**, 3420-3426 (2008).

159. 'Active template synthesis of rotaxanes and molecular shuttles with switchable dynamics via four-component Pd(II)-promoted Michael additions' S M Goldup, D A Leigh, P J Lusby, R T McBurney and A M Z Slawin, *Angew Chem Int Ed*, **47**, 3381-3384 (2008).

158. 'Shaping of a conformationally flexible molecular structure for spectroscopy' A M Rijs, B O Crews, M S de Vries, J S Hannam, D A Leigh, M Fanti, F Zerbetto and W J Buma, *Angew Chem Int Ed*, **47**, 3174-3179 (2008).

157. 'A three state redox-active molecular shuttle that switches in solution and on a surface' G Fioravanti, N Haraszkiwicz, E R Kay, S M Mendoza, C Bruno, M Marcaccio, P G Wiering, F Paolucci, P Rudolf, A M Brouwer and D A Leigh, *J Am Chem Soc*, **130**, 2593-2601 (2008).

[For a highlight of this paper see 'Applied Chemistry Highlights' N P Freestone, *Chem & Ind*, May 2008, 26-28.]

156. 'A chemically-driven molecular information ratchet' M Alvarez-Pérez, S M Goldup, D A Leigh and A M Z Slawin, *J Am Chem Soc*, **130**, 1836-1838 (2008).

[For a highlight of this paper see 'Energy in Motion' D Castelvechi, *Science News*, **173**(8), 120-121 (2008)]

155. 'Beyond switches: Rotaxane- and catenane-based synthetic molecular motors' E R Kay and D A Leigh, *Pure Appl Chem*, **80**, 17-29 (2008).

154. 'Chemically driven artificial molecular machines' J D Crowley, E R Kay and D A Leigh in *Intelligent Materials*, M Shahinpoor and H-J Schneider (eds), p. 1-47, RSC, Cambridge (2008).

## 2007

153. 'Structural dynamics of rotaxanes studied by infrared photon echo spectroscopy' S Yeremenko, O F A Larsen, P Bodis, W J Buma, J S Hannam, D A Leigh and S Woutersen, *Springer Series in Chemical Physics*, **88**, 430-432 (2007).

152. 'A switchable palladium-complexed molecular shuttle and its metastable positional isomers' J D Crowley, D A Leigh, P J Lusby, R T McBurney, L-E Perret-Aebi, C Petzold, A M Z Slawin and M D Symes, *J Am Chem Soc*, **129**, 15085-15090 (2007).

151. 'A metal-complex-tolerant CuAAC 'click' protocol exemplified through the preparation of homo- and mixed-metal-coordinated [2]rotaxanes' D González Cabrera, B D Koivisto and D A Leigh, *Chem Commun*, 4218-4220 (2007).

150. '[2]Rotaxanes through palladium active-template oxidative Heck cross-couplings' J D Crowley, K D Hänni, A-L Lee and D A Leigh, *J Am Chem Soc*, **129**, 12092-12093 (2007).

149. 'Catalytic 'active-metal' template synthesis of [2]rotaxanes, [3]rotaxanes and molecular shuttles, and some observations on the mechanism of the Cu(I)-catalyzed azide-alkyne 1,3-cycloaddition' V Aucagne, J Berná, J D Crowley, S M Goldup, K D Hänni, D A Leigh, P J Lusby, V E Ronaldson, A M Z Slawin, A Viterisi and D B Walker, *J Am Chem Soc*, **129**, 11950-11963 (2007).

148. 'A catalytic palladium active-metal template pathway to [2]rotaxanes' J Berná, J D Crowley, S M Goldup, K D Hänni, A-L Lee, D A Leigh *Angew Chem Int Ed*, **46**, 5709-5713 (2007).

[For a highlight of this paper see 'Palladium-Catalyzed Synthesis of Rotaxanes' T M Swager and R M Moslin, *Synfacts*, 1158 (2007)]

147. 'The effect of solvent upon molecularly thin rotaxane film formation', A A Farrell, E R Kay, G Bottari, D A Leigh and S P Jarvis, *Appl Surf Sci*, **253**, 6090-6095 (2007).

146. 'One template, multiple rings: Controlled iterative addition of macrocycles onto a single binding site rotaxane thread' A-M L Fuller, D A Leigh and P J Lusby, *Angew Chem Int Ed*, **46**, 5015-5019 (2007). ['VIP' paper]

145. 'Hetero-vibrational interactions, cooperative hydrogen bonding and vibrational energy relaxation pathways in a rotaxane' P Bodis, R Timmer, S Yeremendo, W J Buma, J S Hannam, D A Leigh and S Woutersen, *J Phys Chem C*, **111**, 6798-6804 (2007).

144. 'A molecular information ratchet' V Serreli, C-F Lee, E R Kay and D A Leigh, *Nature*, **445**, 523-527 (2007).

[For highlights of this paper see 'Knowledge is power!' (N&V's) A P Davis, *Nature Nanotech*, **2**, 135-136 (2007); 'Demon ratchets up nanotech revolution' *Chemistry World*, 31 Jan 2007; 'Scientists build nanomachine envisaged 150 years ago' *Scientific American*, 31 Jan 2007; 'Tiny engine boosts nanotech hopes' *BBC news*, 1 Feb 2007; '1867 nanomachine now reality' *CNN*, 2 Feb 2007; 'Laws of Nature survive attack by Nano Demon' *Daily Telegraph*, 2 Feb 2007; etc.]

143. 'A rotaxane mimic of the photoactive yellow protein chromophore environment: Effects of hydrogen bonding and mechanical interlocking on a coumaric amide derivative' J Berná, A M Brouwer, S M Fazio, N Haraszkiwicz, D A Leigh and C M Lennon (néé Keaveney), *Chem Commun*, 1910-1912 (2007).

142. 'Coumaric amide rotaxanes: Effects of hydrogen bonding and mechanical interlocking on the photochemistry and photophysics' A M Brouwer, S M Fazio, N Haraszkiwicz, D A Leigh and C M Lennon (néé Keaveney), *Photochem Photobiol Sci*, **6**, 480-486 (2007).

141. 'Amide-based molecular shuttles (2001-2006)' J Berná, G Bottari, D A Leigh and E M Pérez, *Pure Appl Chem*, **79**, 39-54 (2007).

140. 'Extremely strong and readily accessible AAA-DDD triple hydrogen bond complexes' S Djurdjevic, D A Leigh, H McNab, S Parsons, G Teobaldi and F Zerbetto, *J Am Chem Soc*, **129**, 476-477 (2007).

[For a highlight of this paper see: 'Really Strong Triple H-Bonding' *Chem & Eng News*, **85**(2), 44 (2007)]

139. 'Synthetic molecular motors and mechanical machines', E R Kay, D A Leigh and F Zerbetto, *Angew Chem Int Ed*, **46**, 72-191 (2007).

[The longest review ever published by *Angewandte Chemie* (half of a special double issue to celebrate 40 years of supramolecular chemistry and the 20th anniversary of the Pedersen•Cram•Lehn Nobel Prize); Most-accessed *Angewandte Chemie* article Dec 2006-Nov 2007; Most-cited *Angewandte Chemie* article since 2007 (as of 28 May 2012). Source: *Angewandte Chemie*]

## 2006

138. 'Self-organization of nano-lines and dots triggered by a local mechanical stimulus' F Biscarini, M Cavallini, R Kshirsagar, G Bottari, D A Leigh, S León and F Zerbetto, *Proc Natl Acad Sci USA*, **103**, 17650-17654 (2006).

[For a highlight of this paper see: 'Self-assembly: Push to organize' A L Chun, *Nature Nanotech*, **2**, 15 (2007)]

137. 'Switchable dual binding mode molecular shuttle' D A Leigh and A R Thomson, *Org Lett*, **8**, 5377-5379 (2006).

136. 'Adsorption of fumaramide [2]rotaxane and its components on a solid substrate: A coverage-dependent study' C M Whelan, F G Gatti, D A Leigh, S Rapino, F Zerbetto and P Rudolf, *J Phys Chem B*, **110**, 17076-17081 (2006).

135. 'Chemoselective formation of successive triazole linkages in one pot: "Click-click" chemistry' V Aucagne and D A Leigh, *Org Lett*, **8**, 4505-4507 (2006).

[Top ten most-requested Chemistry and Chemistry-related journal article in 4th quarter 2006, *CAS Science Spotlight*]

134. 'Surface enhanced second harmonic generation from macrocycle, catenane and rotaxane thin films: Experiments and theory', I Arfaoui, V Bermúdez, G Bottari, C De Nadai, J-P Jalkanen, F Kajzar, D A Leigh, M Lubomska, S M Mendoza, J Niziol, P Rudolf and F Zerbetto, *J Phys Chem B*, **110**, 7648-7652 (2006).

133. 'Lighting Up Nanomachines', E R Kay and D A Leigh, *Nature*, **440**, 286-287 (2006).

132. 'Dynamic chirality: Molecular shuttles and motors', D A Leigh and E M Pérez, in *Supramolecular Chirality*, M Crego-Calama & D N Reinhoudt (eds.), *Topics Curr Chem*, **265**, 185-208 (2006).

131. 'Beyond switches: Ratcheting a particle energetically uphill with a compartmentalized molecular machine' M N Chatterjee, E R Kay and D A Leigh, *J Am Chem Soc*, **128**, 4058-4073 (2006).

[15th most-cited *J Am Chem Soc* article in 2006]

130. 'Catalytic "click" rotaxanes: A substoichiometric metal-template pathway to mechanically-interlocked architectures' V Aucagne, K D Hänni, D A Leigh, P J Lusby and D B Walker, *J Am Chem Soc*, **128**, 2186-2187 (2006).

129. 'Rotaxanes of cyclic peptides' V Aucagne, D A Leigh, J S Lock and A R Thomson, *J Am Chem Soc*, **128**, 1784-1785 (2006).

[For a highlight of this paper see: 'Peptides Trapped On A Thread', *Chem & Eng News*, Jan 25 (2006)]

128. 'Self-organization of rotaxane thin films into spatially correlated nanostructures: Morphological and structural aspects' J-F Moulin, J C Kengne, R Kshirsagar, M Cavallini, F Biscarini, S Léon, F Zerbetto, G Bottari and D A Leigh, *J Am Chem Soc*, **128**, 526-532 (2006).

127. 'An allosterically regulated molecular shuttle' D S Marlin, D González Cabrera, D A Leigh and A M Z Slawin, *Angew Chem Int Ed*, **45**, 1385-1390 (2006).

126. 'Complexation-induced translational isomerism: Shuttling through step-wise competitive binding' D S Marlin, D González Cabrera, D A Leigh and A M Z Slawin, *Angew Chem Int Ed*, **45**, 77-83 (2006).

## 2005

125. 'Probing the structure of a rotaxane with two-dimensional infrared spectroscopy' O F A Larsen, P Bodis, W J Buma, J S Hannam, D A Leigh and S Woutersen, *Proc Natl Acad Sci USA*, **102**, 13378-13382 (2005).

[For highlights of this paper see: 'Fast Vibrational Coupling' *Science*, **309**, 1967 (2005); 'Coherent femtosecond multidimensional probes of molecular vibrations' (N&V's) S Mukamel and W Zhuang, *Proc Natl Acad Sci USA*, **102**, 13717-13718 (2005); etc.]

124. 'Half-rotation in a [2]catenane via interconvertible Pd(II) coordination modes' D A Leigh, P J Lusby, A M Z Slawin and D B Walker, *Chem Commun*, 4919-4921 (2005).

123. 'Hydrogen bond-assembled synthetic molecular motors and machines' E R Kay and D A Leigh in 'Molecular Machines' T R Kelly (ed.), *Topics Curr Chem*, **262**, 133-177 (2005).

122. 'Conservative and dissipative force Imaging of switchable rotaxanes with frequency modulation atomic force microscopy' A A Farrell, T Fukuma, T Uchihashi, E R Kay, G Bottari, D A Leigh, H Yamada and S P Jarvis, *Phys Rev B*, **72**, 125430 (2005).

121. 'Selecting topology and connectivity through metal-directed macrocyclization reactions: A square planar palladium [2]catenane and two non-interlocked isomers' A-M L Fuller, D A Leigh, P J Lusby, A M Z Slawin and D B Walker, *J Am Chem Soc*, **127**, 12612-12619 (2005).

120. 'Macroscopic transport by synthetic molecular machines' J Berná, D A Leigh, M Lubomska, S M Mendoza, E M Pérez, P Rudolf, G Teobaldi and F Zerbetto, *Nature Mater*, **4**, 704-710 (2005).

[One of the 'Top ten most influential Nature Materials papers of 2005-2006' according to the *Nature Materials* website. For highlights of this paper see: 'Drop by drop', *Nature*, **437**, 4-5 (2005); 'Drop in attendance at motor show' (N&V's), D Fitzmaurice *Nature Mater*, **4**, 657 (2005) etc.]

119. 'Rare and diverse binding modes introduced through mechanical bonding' D A Leigh, P J Lusby, A M Z Slawin and D B Walker, *Angew Chem Int Ed*, **44**, 4557-4564 (2005).

118. 'Patterning through controlled submolecular motion: Rotaxane-based switches and logic gates that function in solution and polymer films', D A Leigh, M Á F Morales, E M Pérez, J K Y Wong, C G Saiz, A M Z Slawin, A J Carmichael, D M Haddleton, A M Brouwer, W J Buma, G W H Worpel, S León and F Zerbetto, *Angew Chem Int Ed*, **44**, 3062-3067 (2005).

[Featured on the front cover, issue 20, May 2005; For highlights of this paper see 'Molecular Memories Start to Gel', *Materials Update*, 26 May 2005; 'Switches Based on Submolecular Movement', *Materials Today*, July 2005 etc.]

117. 'Synthetic molecular machines' E R Kay and D A Leigh in 'Functional Artificial Receptors', T. Schrader, A. D. Hamilton (eds.), Wiley-VCH, Weinheim, 333-406 (2005).

116. 'IRAS investigation of a catenane adsorption on Au(111)' C A Fustin, S Haq, A Wingen, C Grégoire, R Raval, P Dumas, J S Hannam, D A Leigh and P Rudolf, *Surf Sci*, **580**, 57-62 (2005).

## 2004

115. 'A reversible synthetic rotary molecular motor' J V Hernández, E R Kay and D A Leigh, *Science*, **306**, 1532-1537 (2004).

[For highlights of this paper see 'First two-way artificial molecular motor obeys the laws of thermodynamics', *Chemistry World*, January 2005 etc.]

114. 'Shuttling through reversible covalent chemistry' D A Leigh and E M Pérez, *Chem Commun*, 2262-2263 (2004).

113. 'A generic basis for some simple light-operated mechanical molecular machines' E M Pérez, D T F Dryden, D A Leigh, G Teobaldi and F Zerbetto, *J Am Chem Soc*, **126**, 12210-12211 (2004).

112. 'A 3D interlocked structure from a 2D template: Structural requirements for the assembly of a square planar metal-coordinated [2]rotaxane' A-M Fuller, D A Leigh, P J Lusby, I D H Oswald, S Parsons and D B Walker, *Angew Chem Int Ed*, **43**, 3914-3918 (2004).

111. 'Controlled submolecular translational motion in synthesis: A mechanically interlocking auxiliary' J S Hannam, S M Lacy, D A Leigh, C G Saiz, A M Z Slawin and S G Stitchell, *Angew Chem Int Ed*, **43**, 3260-3264 (2004).

[For highlights of this paper see: 'Mechanical Synthesis' *Science*, **305**, 149 (2004) etc.]

110. 'Shuttling through anion recognition' C M Keaveney and D A Leigh, *Angew Chem Int Ed*, **43**, 1222-1224 (2004).

109. 'A simple general ligand system for assembling octahedral metal-rotaxane complexes', L Hogg, D A Leigh, P J Lusby, A Morelli, S Parsons and J K Y Wong, *Angew Chem Int Ed*, **43**, 1218-1221 (2004); ['VIP' paper].

108. 'The mechanism of formation of amide-based interlocked compounds: Prediction of a new rotaxane-forming motif' D A Leigh, A Venturini, A J Wilson, J K Y Wong and F Zerbetto, *Chem Eur J*, **10**, 4960-4969 (2004).

107. 'Structural, electrochemical, and photophysical properties of a molecular shuttle attached to an acid-terminated self-assembled monolayer' F Cecchet, P Rudolf, S Rapino, M Margotti, F Paolucci, J Baggerman, A M Brouwer, E R Kay, J K Y Wong and D A Leigh, *J Phys Chem B*, **108**, 15192-15199 (2004).

106. 'Optical and low frequency electric field testing of the mobility of mobile parts in catenanes and rotaxanes', K Nowicka, P A Chollet, F Kajzar, G Bottari, F G Gatti, D A Leigh and A Miniewicz, *Nonlinear Optics, Quant Optics*, **32**, 175-186 (2004).

105. 'Mechanically linked poly(ethylene terephthalate)' C A Fustin, G J Clarkson, D A Leigh, F Van Hoof, A M Jonas, and C Bailly, *Macromolecules*, **37**, 7884-7892 (2004).

104. 'Solution and solid-state properties of mechanically linked polycarbonates', C A Fustin, C Bailly, G J Clarkson, T H Galow and D A Leigh, *Macromolecules*, **37**, 66-70 (2004).

## 2003

103. 'Unidirectional rotation in a mechanically interlocked molecular rotor', D A Leigh, J K Y Wong, F Dehez and F Zerbetto, *Nature*, **424**, 174-179 (2003).

[For highlights of this paper see: 'Chemistry in motion – unidirectional rotating molecular motors' C. P. Mandl and B. König, *Angew Chem Int Ed*, **35**, 1622-1624 (2004); 'Chemical Highlights of 2003', *Chem & Eng News*, **81**(51), 39-50 (2003); 'Chemical turnstiles', *Science*, **301**, 438-439 (2003); 'Molecular motor has novel three-ring design', *Chem & Eng News*, **81**(28), 14 (2003); etc.]

102. 'Information storage using supramolecular surface patterns' M Cavallini, F Biscarini, S León, F Zerbetto, G Bottari and D A Leigh, *Science*, **299**, 531 (2003).

[For highlights of this paper see: 'Molecular abacus stores abundant information' *Scientific American*, Jan 27, 2003; 'Molecular dots rise for information storage' *Institute of Physics News*, 27 Jan, 2003; 'Molecular abacus' *Materials Today*, March 2003; 'Intelligent molecules for more efficient DVD's', *NBC*, 29 Jan 2003 etc.]

101. 'Entropy-driven translational isomerism: A tristable molecular shuttle' G Bottari, F Dehez, D A Leigh, P J Nash, E M Pérez, J K Y Wong and F Zerbetto, *Angew Chem Int Ed*, **42**, 5886-5889 (2003).

100. 'Rotaxane building blocks bearing blocked isocyanate stoppers - polyrotaxanes through post-assembly chain extension', T J Kidd, T J A Loontjens, D A Leigh and J K Y Wong, *Angew Chem Int Ed*, **42**, 3379-3383 (2003); ['VIP' paper].

99. 'Remarkable positional discrimination in bistable light- and heat- switchable hydrogen-bonded molecular shuttles', A Altieri, G Bottari, F Dehez, D A Leigh, J K Y Wong and F Zerbetto, *Angew Chem Int Ed*, **42**, 2296-2300 (2003); ['Hot' paper].

98. 'Chiroptical switching in a bistable molecular shuttle' G Bottari, D A Leigh and E M Pérez, *J Am Chem Soc*, **125**, 13360-13361 (2003).
97. 'Electrochemically switchable hydrogen-bonded molecular shuttles', A Altieri, F G Gatti, E R Kay, D A Leigh, F Paolucci, A M Z Slawin and J K Y Wong, *J Am Chem Soc*, **125**, 8644-8654 (2003).
96. 'Mechanically linked polycarbonate', C A Fustin, C Bailly, G J Clarkson, P De Groote, T H Galow, D A Leigh, D Robertson, A M Z Slawin and J K Y Wong, *J Am Chem Soc*, **125**, 2200-2207 (2003).
95. 'Photoisomerization of a rotaxane hydrogen bonding template: Light-induced acceleration of a large amplitude rotational motion' F G Gatti, S Leòn, J K Y Wong, G Bottari, A Altieri, M A Farran Morales, S J Teat, C Frochot, D A Leigh, A M Brouwer and F Zerbetto, *Proc Natl Acad Sci USA*, **100**, 10-14 (2003).  
[For highlights of this paper see: 'Nanowheels Get Revved Up', *Science Now*, 23 December 2002; etc.]
94. 'Magic rod' rotaxanes: The hydrogen bond-directed synthesis of molecular shuttles under thermodynamic control, J S Hannam, T J Kidd, D A Leigh and A J Wilson, *Org Lett*, **5**, 1907-1910 (2003).
93. 'A hydrogen bond-assembled fullerene molecular shuttle', T Da Ros, D M Guldi, A Farran Morales, D A Leigh, M Prato and R Turco, *Org Lett*, **5**, 689-691 (2003).
92. 'Rotaxanes - novel photonic molecules', V Bermudez, T Gase, F Kajzar, N Capron, F Zerbetto, F G Gatti, D A Leigh and S Zhang, *Opt Mater*, **21**, 39-44 (2003).
91. 'Grafting of benzylic amide macrocycles onto acid-terminated self-assembled monolayers studied by XPS, RAIRS, and contact angle measurements', F Cecchet, M Pilling, L Hevesi, S Schergna, J K Y Wong, G J Clarkson, D A Leigh and P Rudolf, *J Phys Chem B*, **107**, 10863-10872 (2003).
90. 'Summing Up Ligand Binding Interactions' (N&V), D A Leigh, *Chem & Biol*, **10**, 1143-1144 (2003).
89. 'Synthesis and characterization of mechanically-linked polycarbonates', C-A Fustin, C Bailly, G J Clarkson, P De Groote, T H Galow, D A Leigh, D Robertson, A M Z Slawin and J K Y Wong, *Polymer Preprints*, **44**, 758-759 (2003).
88. 'Photoinduced dynamics in hydrogen-bonded rotaxanes', A M Brouwer, S M Fazio, C Frochot, F G Gatti, D A Leigh, J K Y Wong and G W H Wurpel, *Pure Appl Chem*, **75**, 1055-1060 (2003).
87. 'Molecules in motion: Towards hydrogen bond-assembled molecular machines', D A Leigh in 'Organic Nanophotonics' F Charra, V M Agranovich and F Kajzar (eds.), p. 47-56, Kluwer, Dordrecht, (2003).
- 2002**
86. 'From reactants to products via simple hydrogen-bonding networks: Information transmission in chemical reactions' G Brancato, F Coutrot, D A Leigh, A Murphy, J K Y Wong and F Zerbetto, *Proc Natl Acad Sci USA*, **99**, 4967-4971 (2002).
85. 'Switching 'on' and 'off' the expression of chirality in peptide rotaxanes' M Asakawa, G Brancato, M Fanti, D A Leigh, T Shimizu, A M Z Slawin, J K Y Wong, F Zerbetto, and S Zhang, *J Am Chem Soc*, **124**, 2939-2950 (2002).
84. 'The effect of mechanical interlocking on crystal packing: predictions and testing' F Biscarini, M Cavallini, D A Leigh, S León, S J Teat, J K Y Wong, F Zerbetto, *J Am Chem Soc*, **124**, 225-233 (2002).
83. 'Spontaneous fabrication of microscopic arrays of molecular structures with submicron length scales' M Cavallini, F Biscarini, M Massi, A Farran Morales, D A Leigh and F Zerbetto, *Nano Lett*, **2**, 635-639 (2002).
82. 'The effect of guest inclusion on the crystal packing of p-tert-butylcalix-4-arenes' S Leòn, D A Leigh and F Zerbetto, *Chem Eur J*, **8**, 4854-4866 (2002).
81. 'Solid-state fingerprints of molecular threading detected by inelastic neutron scattering' G Bottari, R Caciuffo, M Fanti, D A Leigh, S F Parker and F Zerbetto, *ChemPhysChem*, 1038-1041 (2002).
80. 'Excited and Ionic States of Formamide: An Excited-state Photoelectron Spectroscopy and ab initio Study' D H A ter Steege, C Lagrost, W J Buma, D A Leigh and F Zerbetto, *J Chem Phys*, **117**, 8270-8280 (2002).
79. 'Effect of Potassium Intercalation on the Electronic and Vibrational Properties of Benzylic Amide [2]Catenane Films' C A Fustin, R Gouttebaron, R Caudano, P Rudolf, D A Leigh, M Fanti, A Krug and F Zerbetto, *Surf Sci*, **515**, 45-52 (2002).
78. 'Adsorption of a Benzylic Amide Macrocyclic on a Solid Substance: XPS and HREELS Characterization of Thin Films Grown on Au(III)' C M Whelan, F Cecchet, R Baxter, F Zerbetto, G J Clarkson, D A Leigh and P Rudolf, *J Phys Chem B*, **106**, 8739-8746 (2002).
77. 'Light-Induced Changes in NO<sub>2</sub>-Substituted Rotaxanes: Switching Behavior in a Mechanically Interlocked Architecture' V Bermudez, P A Chollet, F Kajzar, A Lorin, G Bottari, F G Gatti and D A Leigh, *Mol Cryst Liq Cryst*, **374**, 343-356 (2002).

- 2001**
76. 'Photoinduction of Fast, Reversible Translational Motion in a Hydrogen-Bonded Molecular Shuttle' A M Brouwer, C Frochot, F G Gatti, D A Leigh, L Mottier, F Paolucci, S Roffia, G W H Wurpel, *Science*, **291**, 2124-2128 (2001).

[For highlights of this article see: 'A Light-Driven Linear Motor at the Molecular Level', J-P Sauvage, *Science*, **291**, 2105-2106 (2001) etc.]

75. 'Benzylic Imine Catenates: Readily Accessible Octahedral Analogues of the Sauvage Catenates' D A Leigh, P J Lusby, S J Teat, A J Wilson, J K Y Wong, *Angew Chem Int Ed*, **40**, 1538-1543 (2001)

74. 'Enhanced Hydrogen Bonding Induced by Optical Excitation: Unexpected Subnanosecond Photoinduced Dynamics in a Peptide-based [2]Rotaxane' G W H Wurpel, A M Brouwer, I H M van Stokkum, A Farran and D A Leigh *J Am Chem Soc*, **123**, 11327-11328 (2001).

73. 'Stiff, and Sticky in the Right Places: The Dramatic Influence of Preorganizing Guest Binding Sites on the Hydrogen Bond-Directed Assembly of Rotaxanes', F G Gatti, D A Leigh, S A Nepogodiev, A M Z Slawin, S J Teat, J K Y Wong, *J Am Chem Soc*, **123**, 5983-5989 (2001).

72. 'Quantum-Mechanical Description of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes', D A Leigh, A Troisi, F Zerbetto, *Chem Eur J*, **7**, 1450-1454 (2001).

71. 'The Inelastic Neutron Scattering of Two Benzylic Amide [2]Catenanes' D A Leigh, S F Parker, D Timpel, F Zerbetto, *J Chem Phys*, **114**, 5006-5011 (2001).

70. 'Conformational self-recognition as the origin of dewetting in bistable molecular surfaces', M Cavallini, R Lazzaroni, R Zamboni, F Biscarini, D Timpel, F Zerbetto, G J Clarkson and D A Leigh, *J Phys Chem B*, **105**, 10826-10830 (2001).

69. 'Solid-state optical properties of the methyl-exopyridine-anthracene rotaxane' G Gadret, R Zamboni, P Schouwink, R F Mahrt, J Thies, T Loontjens, and D A Leigh, *Chem Phys*, **269**, 381-388 (2001).

68. 'A High Resolution Electron Energy Loss Spectroscopy Study of the Adsorption of a Benzylic Amide Macrocyclic on Au(111)' C M Whelan, F Cecchet, G J Clarkson, D A Leigh, R Caudano and P Rudolf, *Surf Sci*, **474**, 71-80 (2001).

67. 'Photoemission Study of Pristine and Potassium Intercalated Benzylic Amide [2]Catenane Films', C-A Fustin, R Gouttebaron, C De Nadaï, R Caudano, P Rudolf, F Zerbetto and D A Leigh, *Surf Sci*, **474**, 37-40 (2001).

66. 'Photophysical properties of thin films and solid phase of switchable anthracene-based rotaxanes', G Giro, M Cocchi, V Fattori, G Gadret, G Ruani, M Cavallini, F Biscarini, R Zamboni, T Loontjens, J Thies, D A Leigh, A F Morales and R F Mahrt, *Synthetic Metals*, **122**, 63-65 (2001).

65. 'Excimer-like electroluminescence from thin films of switchable anthracene-based rotaxanes', G Giro, M Cocchi, V Fattori, G Gadret, G Ruani, M Murgia, M Cavallini, F Biscarini, R Zamboni, T Loontjens, J Thies, D A Leigh and A F Morales, *Synthetic Metals*, **122**, 27-29 (2001).

64. 'Optical and electroemission properties of thin films of anthracene-based rotaxanes', G Gadret, G Ruani, M Cavallini, F Biscarini, M Murgia, R Zamboni, G Giro, M Cocchi, V Fattori, T Loontjens, J Thies, D A Leigh, A F Morales and R F Mahrt, *Appl Surf Sci*, **175**, 369-373 (2001).

## 2000

63. 'Reducing Molecular Shuttling to a Single Dimension' D A Leigh, A Troisi, and F Zerbetto, *Angew Chem Int Ed*, **39**, 350-353 (2000).

62. 'Influencing Intramolecular Motion with an Alternating Electric Field' V Bermudez, N Capron, T Gase, F G Gatti, F Kajzar, D A Leigh, F Zerbetto, S Zhang, *Nature*, **406**, 608-611 (2000).

[For highlights of this paper see 'Electric Field Powers Molecular Carousel' *Chem & Eng News*, August 14, 32 (2000) etc.]

61. 'Physical Consequences of a Mechanically Interlocked Architecture: Benzylic Amide Catenane NH Stretching Vibrations as Sensitive Probes for Weakly Hydrogen-Bonding Environments' C-A Fustin, D A Leigh, P Rudolf, D Timpel, F Zerbetto *ChemPhysChem*, 97-100 (2000).

60. 'Nonlinear optical properties of benzylic amide [2]catenanes: a novel versatile photonic material' D Grando, T Gase, F Kajzar, M Fantì, F Zerbetto, A Murphy, D A Leigh *Mol Cryst Liq Cryst*, **353**, 545-559 (2000).

59. 'Self-assembly of Mechanically Interlocked and Threaded Rings: a HREELS and XPS Study of Thiol- Catenane and Rotaxane Molecules on Au(111)' C De Nadaï, C M Whelan, C Perollier, G Clarkson, D A Leigh, R Caudano, P Rudolf, *Surf Sci*, **454-456**, 112-117 (2000).

## 1999

58. 'Smart' Rotaxanes: Shape Memory and Control in Tertiary Amide Peptido[2]rotaxanes' W Clegg, C Gimenez-Saiz, D A Leigh, A Murphy, A M Z Slawin and S J Teat, *J Am Chem Soc*, **121**, 4124-4129 (1999).

57. 'How do Benzylic Amide [2]Catenane Rings Rotate?' M S Deleuze, D A Leigh and F Zerbetto, *J Am Chem Soc*, **121**, 2364-2379 (1999).

56. 'Organic 'Magic Rings' - The Hydrogen Bond-Directed Assembly of Catenanes Under Thermodynamic Control' T J Kidd, D A Leigh and A J Wilson, *J Am Chem Soc*, **121**, 1599-1600 (1999).

55. 'Linear and Unanticipated Second-Order Nonlinear Optical Properties of Benzylic Amide [2]Catenane Thin Films: Evidence of Partial Rotation of the Interlocked Molecular Rings in the Solid State' T Gase, D Grando, P-A Chollet, F Kajzar, A Murphy and D A Leigh, *Adv Mater* **11**, 1303-1306 (1999).

54. 'Electrochemically Induced Dynamics of a Benzylic Amide [2]Catenane' P Ceroni, D A Leigh, L Mottier, F Paolucci, S Roffia, D Tetard and F Zerbetto, *J Phys Chem B*, **103**, 10171-10179 (1999).

53. 'Raman and Far Infrared Characterization of the Simplest Benzylic Amide [2]Catenane' R Zamboni, M Muccini, W Gebauer, F Biscarini, M Murgia, G Ruani, D A Leigh, A Murphy and D Tetard *Synthetic Metals* **102**, 1556-1557 (1999).

52. 'STM Investigation of Flexible Supramolecules: Benzylic Amide [2]Catenanes' F Biscarini, W Gebauer, D DiDomenico, R Zamboni, J I Pascual, D A Leigh, A Murphy and D Tetard *Synthetic Metals* **102**, 1466-1467 (1999).

#### 1998

51. 'Controlling the Frequency of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes' D A Leigh, A Murphy, J P Smart, M S Deleuze, F Zerbetto, *J Am Chem Soc* **120**, 6458-6467 (1998).

50. 'Inelastic Neutron Scattering of Large Molecular Systems: The Case of the Original Benzylic Amide [2]Catenane' R Caciuffo, A Degli Esposti, M S Deleuze, D A Leigh, A Murphy, B Paci, S F Parker and F Zerbetto, *J Chem Phys*, **109**, 11094-11100 (1998).

49. 'Experimental and Theoretical Studies of the Low-lying Electronic States of the Simplest Benzylic Amide [2]Catenane' A M Brouwer, W J Buma, R Caudano, M Fanti, C A Fustin, D A Leigh, A Murphy, P Rudolf, F Zerbetto and J M Zwier, *Chem Phys*, **238**, 421-428 (1998).

48. 'High-Frequency Vibrations of the Simplest Benzylic Amide [2]Catenane' M Fanti, C-A Fustin, D A Leigh, A Murphy, P Rudolf, R Caudano, R Zamboni, F Zerbetto, *J Phys Chem A*, **102**, 5782-5788 (1998).

47. 'Thin Films of a Benzylic Amide [2]Catenane as a Novel Versatile Photonic Material' T Gase, D Grando, P A Chollet, F Kajzar, A Lorin, D Tetard and D A Leigh *Photonics Sci News*, **3**, 16-21 (1998).  
[Front cover 'Benzylic Amide Catenanes as Novel Versatile Photonic Materials' *Photonics Sci News*, issue 4, **3**, 1998]

46. 'Growth and Characterization of Benzylic Amide [2]Catenane Thin Films' C A Fustin, P Rudolf, A F Taminiaux, F Zerbetto, D A Leigh and R Caudano, *Thin Solid Films*, **329**, 321-325 (1998).

#### 1997

45. 'Studies of Multiple-chain Alkylaminomethyl p-Cyanophenol Derivatives for Langmuir-Blodgett Films' K A Longstaff, D A Leigh and R W Munn *Adv Mat Optics Elec*, **7**, 295-305 (1997).

44. 'Peptide-based Molecular Shuttles' A S Lane, D A Leigh and A Murphy *J Am Chem Soc*, **119**, 11092-11093 (1997).  
[For highlights of this paper see 'Molecular Shuttles', *Science News*, May 1997 etc.]

43. 'Glycylglycine Rotaxanes - The Hydrogen Bond Directed Assembly of Synthetic Peptide Rotaxanes' D A Leigh, A Murphy, J P Smart and A M Z Slawin *Angew Chem, Int Ed Engl*, **36**, 728-732 (1997).

#### 1996

42. 'Crystallization-Resistant Photorefractive Polymer Composite with High Diffraction Efficiency and Reproducibility' A M Cox, R D Blackburn, D P West, T A King, F A Wade and D A Leigh, *Appl Phys Lett*, **68**, 2801-2803 (1996)

41. 'The Synthesis and Solubilization of Amide Macrocycles via Rotaxane Formation' A G Johnston, D A Leigh, A Murphy, J P Smart and M D Deegan *J Am Chem Soc*, **118**, 10662-10663 (1996)

40. 'The Programmed Assembly-Controlled Disassembly of [2]Rotaxanes as a Strategy in Synthesis: The Preparation of a Chemical Sensor for CO<sub>2</sub>' A G Johnston, D A Leigh, A Murphy and J P Smart, *Bull Chem Soc Belg*, **105**, 721-727 (1996)

39. 'Catenane Chameleons: Environment-Sensitive Translational Isomerism in Amphiphilic Benzylic Amide [2]Catenanes' D A Leigh, K Moody, J P Smart, K J Watson and A M Z Slawin, *Angew Chem, Int Ed Engl*, **35**, 306-310 (1996).

38. 'Fast Atom Bombardment Mass Spectrometry as a Tool for the Rapid Determination of Enantioselective Binding of Methylated Cyclodextrins' S N Davey, D A Leigh, J P Smart, L W Tetler and A M Truscello, *Carbohydr Res*, **290**, 117-123 (1996).

#### 1995

37. 'Structurally Diverse and Dynamically Versatile Benzylic Amide [2]Catenanes Assembled Directly from Commercially Available Precursors' A G Johnston, D A Leigh, L Nezhat, J P Smart and M D Deegan, *Angew Chem, Int Ed Engl*, **34**, 1212-1216 (1995).

36. 'Facile Synthesis and Solid State Structure of a Benzylic Amide [2]Catenane' A G Johnston, D A Leigh, R J Pritchard and M D Deegan, *Angew Chem, Int Ed Engl*, **34**, 1209-1212 (1995).

[Front cover, *Angew Chem* and *Angew Chem, Int Ed Engl*, issue 11, **34**, 1995. For highlights of this paper see 'An Unexpected Chain of Events' *Lab News*, April 1995, 'Organic Chemistry Highlights' *Chem & Ind*, June 1995, etc.]

35. 'Intermolecular Aglycon Transfer of Ethyl 1-Thiorhamnopyranosides under Koenigs-Knorr Glycosylation Conditions' D A Leigh, J P Smart and A M Truscillo, *Carbohydr Res*, **276**, 417-424 (1995).

34. 'Second Harmonic Generation from Langmuir-Blodgett Films of Fullerene Azacrown Ethers' D A Leigh, F Wade, T A King, D West and G S Bahra, *Langmuir*, **11**, 2334-2336 (1995).

#### 1994

33. 'Kinetically-controlled Regioselective Silylation of Polyol's via Dibutylstannylendiyl Acetals' D A Leigh, R P Martin, J P Smart and A M Truscillo, *J Chem Soc, Chem Commun*, 1373-1374 (1994).

32. ' $C_{60}$ -Azacrown Ethers: The First Monoaminated Fullerene Derivatives' S N Davey, D A Leigh, A E Moody, L W Tetler and F A Wade, *J Chem Soc, Chem Commun*, 397-398 (1994)

31. 'Unusual Host-Guest  $\pi$ -Arene...H bonding in a 'Hooded' Cavitand: The First Solid-state Structure of a Calix[4]resorcinarene with Underivatised Hydroxy Groups' D A Leigh, P Linnane, R G Pritchard and G Jackson, *J Chem Soc, Chem Commun*, 389-340 (1994).

30. 'Endohedral Complexation of Helium Atoms by Derivatised Fullerenes' S N Davey, D A Leigh, A E Moody and L W Tetler, *J Chem Soc, Chem Commun*, 7-8 (1994).

29. '2,7-Dimethyl-3,5-octadiyne-2,7-diol Dichloromethane Solvate: A Clathrate Comprising Hydrogen-Bonded Supramolecular Tunnels Containing Dichloromethane Guest Molecules' D A Leigh, A E Moody and R G Pritchard, *Acta Cryst*, **C50**, 129-131 (1994).

#### 1993

28. 'The Regioselective tert-Butyldimethylsilylation of the 6'-hydroxyl group of Lactose Derivatives via their Dibutylstannylene Acetals' A Glen, D A Leigh, R P Martin, J P Smart and A M Truscillo, *Carbohydrate Res*, **248**, 365-369 (1993).

[For a highlight of this paper see 'New Properties of Stannylenes: The Regioselective tert-Butyldimethylsilylation of the 6'-hydroxyl group of Lactose Derivatives via their Dibutylstannylene Acetals', *Chemtracts - Org Chem*, 315-319 (1993)]

27. 'The Confinement of Buckminsterfullerene in One-dimensional Channels', M W Anderson, J Shi, D A Leigh, A E Moody, F A Wade, B Hamilton and S W Carr, *J Chem Soc, Chem Commun*, 533-536 (1993).

[For highlights of this paper see 'Bottle and Glow Fullerenes' *Science*, **258**, 1886 (1993), 'Making Light of Spherical Chemistry' *Chem & Ind*, 443-444 (1993), 'Rainbow-Coloured Buckyballs Light Up the Lab' *New Scientist*, 15, 1st May 1993, 'Laser-excited Confined Buckyballs Emit White Light' *Laser Focus World*, **29**, 15 (1993), 'Mineral Brings a Glow to Buckyballs' *Education in Chem*, 165 (1993) etc]

26. 'Broad-band Visible Light Emission from  $C_{60}$  Molecules Confined in Molecular Cage Materials' B Hamilton, J S Rimmer, M W Anderson and D A Leigh, *Adv Mater*, **5**, 583-585 (1993).

25. 'Unorthodox Rate Enhancement in the Mannich Reaction of para-Substituted Phenols Containing Electron-Withdrawing Groups' D A Leigh, P Linnane and G Jackson, *Tetrahedron Lett*, **34**, 5639-5640 (1993).

24. 'Mass Spectrometry of Aminated Fullerene Derivatives' S N Davey, D A Leigh, A E Moody and L W Tetler, *Org Mass Spec*, **28**, 559-563 (1993).

23. 'Design of Langmuir-Blodgett Films for Nonlinear Optics' A Baggaley, M Bishop, J H R Clarke, L E Davis, T A King, D A Leigh, F R Mayers, A Mohebati, R W Munn, M M Shabat, O Szczur, D West and J O Williams, *Mol Cryst Liq Cryst*, **235**, 201-208 (1993).

#### 1992

22. 'A Novel Synthesis of Substituted 12-H-Quino-(2,1-B)(1,3)-Benzodiazepin-4-one Derivatives', M C Aversa, P Bonaccorsi, P Giannetto, R Pritchard, B Beagley, A Truscillo, and D A Leigh, *J Heterocyclic Chem*, **28**, 318-323 (1992).

#### 1990

21. 'The In Situ Activation of Thioglycosides with Bromine: An Improved Glycosylation Method', J O Kihlberg, D A Leigh, and D R Bundle, *J Org Chem*, **55**, 2860-2863 (1990).

#### 1989

20. 'Conformational Analysis of Some 11,12-Dihydrodibenz[B,F][1,5]-oxazocin-6-one Derivatives by NMR Spectroscopy', M C Aversa, P Bonaccorsi, P Giannetto, and D A Leigh, *Tetrahedron*, **45**, 6857-6866 (1989).

19. 'Cycloaddition Reactions of 2,3-Dihydro-1H-1,4-diazepines with Nitrile Oxides and Imines. Synthesis of bis[1,2,4]Oxadiazolo- and bis[1,2,4]Triazolol[1,4]diazepine Derivatives', M C Aversa, P Bonaccorsi, P Giannetto, and D A Leigh, *J Heterocyclic Chem*, **26**, 1619-1622 (1989).

#### 1988



18. 'The Complexation Properties of Some Unnatural and Natural Macrocyclic Trichothecenes', D W Anderson, P R Ashton, R M Black, D A Leigh, A M Z Slawin, J F Stoddart, and D J Williams, *J Chem Soc, Chem Commun*, 904-908 (1988).

#### 1987

17. 'The Facile Conversion of T-2 Toxin and Neosolaniol into Anguidine', D W Anderson, R M Black, D A Leigh, J F Stoddart, and N E Williams, *Tetrahedron Letts*, **28**, 2661-2662 (1987).

16. 'Novel 3,4- and 8,15-Polyether Analogues of Macrocyclic Trichothecenes', D W Anderson, R M Black, D A Leigh, and J F Stoddart, *Tetrahedron Letts*, **28**, 2657-2660 (1987).

15. 'Novel 4,15-Polyether Analogues of Macrocyclic Trichothecenes', D W Anderson, R M Black, D A Leigh, and J F Stoddart, *Tetrahedron Letts*, **28**, 2653-2656 (1987).

#### Journal Papers – Not Refereed

14. 'Molecular Tailoring: The Made-to-Measure Properties of Rotaxanes' D A Leigh and A Murphy, *Chem & Ind*, 178-183 (1999).

[Front cover 'Stitched to Order: Rotaxanes offer Bespoke Molecules' *Chem & Ind*, issue 5, 1 March 1999]

#### Conference Papers – Refereed

13. 'Improved Second Harmonic Generation from Langmuir-Blodgett Films of an Azacrown Ether Fullerene Derivative' D A Leigh, F Wade, T A King, D West and G S Bahra, *Mat Res Soc Symp Proc*, **349**, 343-348 (1994)

#### Conference Papers – Not Refereed

12. 'Mechanically-Linked Macromolecules' G J Clarkson & D A Leigh in 'Emerging Themes in Polymer Science', Ed. A J Ryan, Royal Society of Chemistry, Cambridge, pp 299-306 (2001)

#### Other Publications

##### Patents

11. 'Procedure for the Storage of Information at Extremely High Density on Thin Films of Bistable Molecules', F. Biscarini, M. Cavallini, D A Leigh and F. Zerbetto, Patent application No. BO2002/12/4, 4th Dec 2002.

10. 'Intermediates for manufacture of polymers containing rotaxanes having a cyclotetraamide ring in main chains', M. Asakawa, A. Murphy, D. A. Leigh, T. Shimizu, Jpn. Kokai Tokkyo Koho (2001). Patent application No. JP2001002663, Tokyo, 9th Jan 2001.

9. 'Crystallization-Resistant Photorefractive Materials' A M Cox, F A Wade, R D Blackburn, D P West, D A Leigh and T A King, UK patent no 9609876, 11 May, 1996.

8. 'Polymers for the Decaffeination of Green Coffee Extract' P Hay, D A Leigh and R Liardon, Europatent No. 95203394.2, 7 Dec 1995

7. 'Mannich base Wax Crystal Modifying Agents' D P Linnane, D A Leigh and G Jackson, Exxon UK patent 3476334, 1993.

6. 'Fullerenes: A Light Source Material', M W Anderson, B Hamilton and D A Leigh, UK patent no. 9225831, 10 Dec 1992.

##### Book chapters

5. 'Molecules in Motion: Towards Hydrogen Bond-Assembled Molecular Machines', D A Leigh in 'Organic Nanophotonics' F Charra, V M Agranovich and F Kajzar (eds.), p. 47-56, Kluwer, Dordrecht, (2003).

4. 'Oligomeric and Polymeric Catenanes' D A Leigh and R A Smith in 'Cyclic Polymers' (2nd Edition), J A Semlyen (Ed), 561-600, Kluwer, Dordrecht (2000).

3. 'Make me a Molecule' S E Gibson, K J Hale, D A Leigh, N K Terrett and J Williams in 'The Age of the Molecule' Ed. N Hall, pp 13-44, RSC, Cambridge, (1999) and 'Make me a Molecule' S E Gibson, K J Hale, D A Leigh, N K Terrett, J Williams in 'Cutting Edge Chemistry', Ed. T. Lister, S. Aldridge, J. Johnstone and C. Osborne, pp 15-32, RSC, Cambridge (2001).

2. 'Study of Energy Gap and Electronic Transitions in Model Polymer systems: Electronic vs. Optical Excitations' J J Pireaux, G Gensterblum, C Grégoire, B Y Han, K Hevesi, C A Fustin, P Rudolf, L M Yu, R Caudano, D A Leigh and F Zerbetto, *Sci Tech Polymers and Adv Mater* (Ed. P N Prasad), Plenum Press, New York (1998).

1. 'From Catenanes to Mechanically-linked Polymers' G J Clarkson, D A Leigh and R A Smith, *Curr Opin Solid State & Mater Sci* **3**, 579-584 (1998).