Curriculum Vitae – Dr. Duncan John Mowbray

Department of Physics
School of Physical Sciences and Nanotechnology
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Gender: Male
Born: 18/08/76, Wingham, Canada
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Professional Appointment

- Associate Professor (Sep. 2016 – present)
  Department of Physics, School of Physical Sciences and Nanotechnology, **Yachay Tech University**

Education

- Doctor of Philosophy Applied Mathematics (Jan. 2004 – Jan. 2007)
  "Hydrodynamic Modelling of the Electronic Response of Carbon Nanotubes"
  Prof. Zoran L. Mišković and Prof. Frank O. Goodman, **University of Waterloo**
- Master of Science Physics (Sep. 2000 – May 2003)
  "Coefficient Based Simulations of Quantum Algorithms"
  Prof. Robert B. Mann, **University of Waterloo**
- Bachelor of Science (Sep. 1995 – Apr. 2000)
  Honours Physics (Dean's Honours List) **University of Waterloo**
- Bachelor of Mathematics (Sep. 1995 – Apr. 2000)
  Honours Applied Mathematics - Cooperative Program (With Distinction) **University of Waterloo**

Scientific Output (main)
63 refereed publications (**19** as first author) and **3** book chapters with **1399** citations (23 per article) and a *h*-index of **22** in journals such as *Science*, *J. Am. Chem. Soc.* (2), *ACS Nano* (3), *J. Phys. Chem. Lett.*, *J. Phys. Chem. C* (10), *J. Chem. Theory Comput*. (3), *ACS Catalysis*, *Phys. Rev. A* (4), *Phys. Rev. B* (13), *J. Catal.*, *New J. Phys.*, *J. Chem. Phys.* (2) and *Nanotechnology*; contributions to 19 international conferences, with 7 oral presentations, 17 poster presentations, and 12 invited talks. ResearcherID: A-5531-2010

Research Interests

Developing *ab initio* methods to describe a wide variety of sub-areas within nanoscience.

- Photovoltaics: Optical absorption and electon-hole separation at molecule/metal oxide interfaces
- Photocatalysis: Band gap engineering of metal oxides using nanostructure and doping
- Nanosensors: Functionalization of carbon nanotubes for conductometric gas sensing
- Nanoelectronics: Functionalization of molecular and nanotube based semiconductors
- Plasmonics: Dynamical response of carbon nanotubes to external fields
- Heterogeneous Catalysis: Metal clusters, nanoparticles, stepped, and kinked surfaces
- Spectroscopy: Dielectric response of dyes, doped carbon nanotubes and graphene

Expertise

- *Many-body quasiparticle G_0W_0 electronic structure and TDDFT-RPA loss function calculations.*
- *Charge transport calculations with the non-equilibrium Green's function methodology.*
- *Ab initio DFT calculations using localized basis set (SIESTA, GPAW), plane wave (DACAPO, VASP), and grid based (GPAW) codes.*
- *Microkinetic modelling based on DFT energetics.*
- *Software development using Python, Matlab, C++, Java, Perl, and Fortran.*

Academic Work Experience

- Juan de la Cierva Research Fellow (Apr. 2011 – Dec. 2015)
  Project: "First principles modelling of low dimensional systems for nanoelectronics, nanosensing, and photocatalysis", Prof. Angel Rubio and Prof. Stefan Kurth
  Nano-bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) Scientific Development Center, Departamento de Física de Materiales, **Universidad del País Vasco** (UPV/EHU).
- Postdoctoral Researcher (Feb. 2010 – Apr. 2011)
  Project: "Time-resolved oxide mediated photocatalysis", Prof Angel Rubio
  Nano-bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) Scientific Development Center, **Donostia International Physics Center** (DIPC).

Academic Work Experience (continued)

- Postdoctoral Researcher (Dec. 2009 – Jan. 2010)
  Project: "Optical excitation energies and photocatalytic activity of doped and undoped metal oxide nanostructures", Prof. Angel Rubio
  HPC-Europa2 (Pan-European Research Infrastructure on High Performance)
  Nano-bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) Scientific Development Center, Depto. Física de Materiales, **Universidad del País Vasco** (UPV/EHU).
- Postdoctoral Researcher (Jun. 2007 – Sep. 2009)
  Prof. Kristian S. Thygesen, Prof. Karsten W. Jacobsen, and Prof. Jens K. Nørskov
  Center for Atomic-scale Materials Design (CAMd), Department of Physics, **Technical University of Denmark** (DTU). Developed multi-terminal transport code within the non-equilibrium Green's function formalism. Experienced modeler of nanostructures using SIESTA, DACAPO, and GPAW density functional theory codes.
- Referee *Nat. Phys., Nat. Comm., Phys. Rev. Lett., Phys. Rev. B, J. Am. Chem. Soc., J. Phys. Chem., Nanotechnology, J. Modern Optics, EJP, J. Phys.: Condens. Matter, Phys. Lett. A, Physica E, Solid State Sciences, Comp. Mat. Sci., Acta Chimica Slovenica*

Teaching and Supervisory Experience

- Research Supervisor (2005 – Present)
  Depto. Física de Materiales, **Universidad del País Vasco** (UPV/EHU)
  Center for Atomic-scale Materials Design (CAMd), **Technical University of Denmark** (DTU)
  Department of Applied Mathematics, **University of Waterloo**
  Co-supervision of Livia Glanzmann (Ph.D. Jan. 2017) "Modelling of Polymer–Carbon Nanotube Heterojunctions for Photovoltaic Applications" and Iker Larraza Arocena (Master's in Nanoscience 2011) "Modeling Molecular Electrons: Applications to Chemical Sensors". Active involvement in the supervision of a further 12 Ph.D., 2 M.Sc., and 4 B.Sc. candidates. Participation included the direction and development of research projects yielding 11 publications and reviewing the content of 7 theses.
- Course Lecturer (2006, 2010, 2011, 2016 – Present)
  School of Physical Sciences and Nanotechnology, **Yachay Tech University** (YT)
  "Mathematical Physics I", Semester V of Physics and Nanotechnology Careers (Fall 2016, Spring 2017)
  Depto. Física de Materiales, **Universidad del País Vasco** (UPV/EHU)
  "Nanostructural Properties", Masters in Nanoscience (2011)
  "Low Dimensional Systems and Nanostructures", Masters in Nanoscience (2010)
  Department of Applied Mathematics, **University of Waterloo**
  "Differential Equations for Physics and Chemistry" (2006)
  Gave lectures of 4 hours/week, authored course notes, designed and marked assignments, composed and marked midterm tests and final examinations, and was solely responsible for course content.
- Teacher's Assistant (1999 – 2007)
  Department of Physics and Department of Applied Mathematics, **University of Waterloo**
  Gave tutorials, marked assignments and examinations, and acted as lab instructor for mathematics, physics, chemistry, biology, and engineering students on various topics within physics and applied mathematics at all levels from first year undergraduates to graduate students.

Relevant Industrial Experience

- Software Designer (1996 – 1999)
  Thinkage Ltd., Kitchener, Ontario, Canada. Worked independently designing and implementing software applications. Experienced Python, Matlab, C++, Java, Perl, and Fortran developer.

Scholarships & Academic Awards

2010 Juan de la Cierva Fellow Sub-programme of the Spanish Ministry for Science & Innovation	2011-2014	25,000.00 € /yr
AMICI Young Scientist Support Fund Grant	2010	400.00 €
HPC Europa2 Transnational Access research visit programme	2009	3,500.00 €
Ontario Graduate Scholarship in Science and Technology	2001, '05, '06	$15,000.00
University of Waterloo Graduate Scholarship	2000, '01, '03, '04	$4,500.00

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List of Publications (ordered by number of citations)

[1] "Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions", D. G. de Oteyza, P. Gorman, Y.-C. Chen, S. Wickenburg, A. Riss, D. J. Mowbray, G. Etkin, Z. Pedramrazi, H.-Z. Tsai, A. Rubio, M. F. Crommie, and F. R. Fischer, *Science*, **340**, 1434 (2013), doi:10.1126/science.1238187. IF 31.477, Cites **162**.

[2] "Trends in CO oxidation rates for metal nanoparticles and close-packed, stepped, and kinked surfaces", T. Jiang, D. J. Mowbray, S. Dobrin, H. Falsig, B. Hvolbæk, T. Bligaard, and J. K. Nørskov, *J. Phys. Chem. C* **113**, 10548 (2009), doi:10.1021/jp811185g. IF 4.835, Cites **134**.

[3] "Influence of functional groups on charge transport in molecular junctions", D. J. Mowbray, G. Jones, and K. S. Thygesen, *J. Chem. Phys.* **128**, 111103 (2008), doi:10.1063/1.2894544. IF 3.122, Cites **82**.

[4] "Stability and electronic properties of TiO_2 nanostructures with and without B and N doping", D. J. Mowbray, J. I. Martinez, J. M. García Lastra, K. S. Thygesen, and K.W. Jacobsen, *J. Phys. Chem. C* **113**, 12301 (2009), doi:10.1021/jp904672p. IF 4.835, Cites **70**.

[5] "Interactions of fast ions with carbon nanotubes: two-fluid model", D. J. Mowbray, Z. L. Mišković, F. O. Goodman, and Y.-N. Wang, *Phys. Rev. B* **70**, 195418 (2004), doi:10.1103/PhysRevB.70.195418. IF 3.664, Cites **70**.

[6] "Density functional theory based screening of novel alkali-transition metal borohydrides: A computational materials design project", J. S. Hummelshøj, *et al. J. Chem. Phys.* **131**, 014101 (2009), doi:10.1063/1.3148892. IF 3.122, Cites **54**.

[7] "Ion interactions with carbon nanotubes in dielectric media", D. J. Mowbray, Z. L. Mišković, and F. O. Goodman, *Phys. Rev. B* **74**, 195435 (2006), doi:10.1103/PhysRevB.74.195435. IF 3.664, Cites **52**.

[8] "Influence of O_2 and N_2 on the conductivity of carbon nanotube networks", D. J. Mowbray, C. Morgan, and K. S. Thygesen, *Phys. Rev. B* **79**, 195431 (2009), doi:10.1103/PhysRevB.79.195431. IF 3.664, Cites **43**.

[9] "Influence of the dynamical image potential on the rainbows in ion channeling through short carbon nanotubes", D. Borka, S. Petrović, N. Nešković, D. J. Mowbray, and Z. L. Mišković, *Phys. Rev. A* **73**, 062902 (2006), doi:10.1103/PhysRevA.73.062902. IF 2.991, Cites **42**.

[10]"Understanding energy-level alignment in donor-acceptor/metal interfaces from core-level shifts", A. El-Sayed, P. Borghetti, E. Goiri, C. Rogero, L. Floreano, G. Lovat, D. J. Mowbray, J. L. Cabellos, Y. Wakayama, A. Rubio, J. E. Ortega, and D. G. de Oteyza, *ACS Nano* **7**, 6914 (2013), doi:10.1021/nn4020888. IF 12.033, Cites **40**.

[11]"Plasmon excitations on a single-wall carbon nanotube by external charges: two-dimensional, two-fluid hydrodynamic model", D. J. Mowbray, S. Segui, J. Gervasoni, Z. L. Mišković, and N. R. Arista, *Phys. Rev. B* **82**, 035405 (2010), doi:10.1103/PhysRevB.82.035405. IF 3.664, Cites **36**.

[12]"Level alignment of a prototypical photocatalytic system: Methanol on TiO_2(110)", A. Migani, D. J. Mowbray, A. Iacomino, J. Zhao, H. Petek, and A. Rubio, *J. Am. Chem. Soc.* **135**, 11429 (2013) doi:10.1021/ja4036994, arXiv:1308.5284. IF 11.444, Cites **36**.

[13]"Comparative study of anchoring groups for molecular electronics: Structure and conductance of Au-S-Au and Au-NH_2-Au junctions", I. S. Kristensen, D. J. Mowbray, K. S. Thygesen, and K. W. Jacobsen, *J. Phys.: Condens. Matter* **20**, 374101 (2008), doi:10.1088/0953-8984/20/37/374101. IF 2.223, Cites **35**.

[14]"Trends in metal oxide stability for nanorods, nanotubes, and surfaces", D. J. Mowbray, J. I. Martínez, F. Calle-Vallejo, J. Rossmeisl, K. S. Thygesen, K. W. Jacobsen, and J. K. Nørskov, *J. Phys. Chem. C* **115**, 2244 (2011), doi:10.1021/jp110489u. IF 4.835, Cites **34**.

[15]"Self blocking of CO-dissociation on a stepped ruthenium surface", S. B. Vendelbo, M. Johansson, D. J. Mowbray, M. P. Andersson, F. Abild-Pedersen, J. H. Nielsen, J. K. Nørskov and I. Chorkendorff, *Top. Cat*al. 53, 357 (2010), doi:10.1007/s11244-010-9445-4. IF 2.608, Cites **33**.

[16]"Solid-state reactions in binary molecular assemblies of F_{16}CuPc and pentacene", Y. Wakayama, D. G. de Orteyza, J. M. García-Lastra, and D. J. Mowbray, *ACS Nano* **5**, 581 (2010), doi:10.1021/nn102887x. IF 12.033, Cites **30**.

[17]"Quasiparticle level alignment for photocatalytic interfaces", A. Migani, D. J. Mowbray, J. Zhao, H. Petek, and A. Rubio *J. Chem. Theory Comput.* **10**, 2103 (2014), doi:10.1021/ct500087v, arXiv:1404.5166. IF 5.310, Cites **27**.

[18]"Understanding Charge Transfer in Donor-Acceptor/Metal Systems: A Combined Theoretical and Experimental Study", J. L. Cabellos, D. J. Mowbray, E. Goiri, A. El-Sayed, L. Floreano, D. G. de Oteyza, C. Rogero, J. E. Ortega, and A. Rubio, *J. Phys. Chem. C*, **116**, 17991 (2012), doi:10.1021/jp3004213.

List of Publications (continued)

IF 4.835, Cites **26**.

[19]"Anomalous insulator metal transition in boron nitride-graphene hybrid atomic layers", L. Song, L. Balicas, D. J. Mowbray, R. B. Capaz, K. Storr, L. Ci, D. Jariwala, S. Kurth, S. G. Louie, A. Rubio, and P. M. Ajayan, *Phys. Rev. B*, **86**, 075429 (2012), doi:10.1103/PhysRevB.86.075429 arXiv:1105.1876. IF 3.664, Cites **26**, Featured in Kaleidoscope (Aug. 2012).

[20]"Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes", J. M. García-Lastra, D. J. Mowbray, K. S. Thygesen, A. Rubio, and K. W. Jacobsen, *Phys. Rev. B* **81**, 245429 (2010), doi:10.1103/PhysRevB.81.245429. IF 3.664, Cites **25**.

[21]"Dynamic interactions of fast ions with carbon nanotubes", D. J. Mowbray, S. Chung, Z. L. Mišković, F. O. Goodman, and Y.-N. Wang, *Nucl. Instrum. & Methods Phys. Res. B* **230**, 142 (2005), doi:10.1016/j.nimb.2004.12.032. Cites **23**.

[22]"Wake effect in interactions of fast ions with carbon nanotubes", D. J. Mowbray, Z. L. Mišković, F. O. Goodman, and Y.-N. Wang, *Phys. Lett. A* **329**, 94 (2004), doi:10.1016/j.physleta.2004.06.090. Cites **23**.

[23]"Scanning tunneling microscopy evidence for the dissociation of carbon monoxide on ruthenium steps", Y. Tison, K. Nielsen, D. J. Mowbray, L. Bech, C. Holse, F. Calle-Vallejo, K. Andersen, J. J. Mortensen, K. W. Jacobsen, and J. H. Nielsen, *J. Phys. Chem. C*, **116**, 14350 (2012), doi:10.1021/jp302424g. IF 4.835, Cites **17**.

[24]"Dynamic polarization effects on the angular distributions of protons channeled through carbon nanotubes in dielectric media", D. Borka, D. J. Mowbray, Z. L. Mišković, S. Petrovć, and N. Neškovć, *Phys. Rev. A* **77**, 032903 (2008), doi:10.1103/PhysRevA.77.032903. IF 2.991, Cites **16**.

[25]"Comparing Quasiparticle H_2O Level Alignment on Anatase and Rutile TiO_2" H. Sun, D. J. Mowbray, A. Migani, J. Zhao, H. Petek, and A. Rubio, *ACS Catalysis* **5**, 4242 (2015), doi:10.1021/acscatal.5b00529, arXiv:1506.04695. IF 7.572, Cites 16.

[26]"Oxidation of CO and H_2 by O_2 and N_2O on gold nanoparticles in microreactors", G. Walther, D. J. Mowbray, T. Jiang, G. Jones, S. Jensen, U. Quaade, and S. Horch, *J. Catal*. **280**, 86 (2008), doi:10.1016/j.jcat.2008.09.003. IF 6.073, Cites **15**.

[27]"Supramolecular Environment-Dependent Electronic Properties of Metal-Organic Interfaces", A. El-Sayed, D. J. Mowbray, J. M. Garcia-Lastra, C. Rogero, E. Goiri, P. Borghetti, A. Turak, B. P. Doyle, M. Dell'Angela, L. Floreano, Y. Wakayama, A. Rubio, J. E. Ortega, and D. G. de Oteyza, *J. Phys. Chem. C*, **116**, 4780 (2012), doi:10.1021/jp211749g. IF 4.835, Cites **15**.

[28]"Photo-induced C-C reactions on insulators towards photolithography of graphene nanoarchitectures", C.-A. Palma, K. Diller, R. Berger, A. Welle, J. Björk, J. L. Cabellos, D. J. Mowbray, A. C. Papageorgiou, N. P. Ivleva, S. Matich, E. Margapoti, R. Niessner, B. Menges, J. Reichert, X.L. Feng, H. J. Räder, F. Klappenberger, A. Rubio, K. Müllen, and J. V. Barth, *J. Am. Chem. Soc.* 136, 4651 (2014), doi:10.1021/ja412868w. IF 11.444, Cites **14**.

[29]"Dynamic interactions of fast ions with multiwalled carbon nanotubes", S. Chung, D. J. Mowbray, Z. L. Mišković, F. O. Goodman, and Y.-N. Wang, *Radiation Phys. Chem.* **76**, 524 (2007), doi:10.1016/j.radphyschem.2005.09.020. Cites **12**.

[30]"Quasiparticle interfacial level alignment of highly hybridized frontier levels: H_2O on TiO_2(110)", A. Migani, D. J. Mowbray, J. Zhao, and H. Petek, *J. Chem. Theory Comput.*, **11**, 239 (2014), doi:10.1021/ct500779s, arXiv:1501.03533. IF 5.310, Cites **12**.

[31]"TDDFT study of time-dependent and static screening in graphene", V. Despoja, D. J. Mowbray, D. Vlahović, and L. Marušić, *Phys. Rev. B*, **86**, 195429 (Nov. 2012), doi:10.1103/PhysRevB.86.195429. IF 3.664, Cites **12**.

[32]"Revealing the adsorption mechanisms of nitroxides on ultra-pure, metallicity-sorted carbon nanotubes", G. Ruiz-Soria, A Pérez Paz, M. Sauer, D. J. Mowbray, P. Lacovig, M. Dalmiglio, S. Lizzit, K. Yanagi, A. Rubio, A. Goldoni, P. Ayala, and T. Pichler ACS Nano 8, 1375 (2014), doi:10.1021/nn405114z. IF 12.033, Cites **12**.

[33]"Time-Dependent Density-Functional Theory of Strong-Field Ionization of Atoms under Soft X-Rays", A. Crawford-Uranga, U. De Giovannini, E. Räsänen, M. J. T. Oliveira, D. J. Mowbray, G. M. Nikolopoulos, E. Karamatskos, D. Markellos, P. Lambropoulos, S. Kurth, and A. Rubio *Phys. Rev. A* **90**, 033412 (2014), doi:10.1103/PhysRevA.90.033412, arXiv:1408.6067. IF 2.991, Cites **12**.

[34]"Combined experimental and ab-initio study of the electronic structure of narrow diameter single wall carbon nanotube buckypaper with predominant (6,4),(6,5) chirality", K. De Blauwe, D. J. Mowbray, Y.

List of Publications (continued)

Miyata, P. Ayala, H. Shiozawa, A. Rubio, P. Hoffmann, H. Kataura, and T. Pichler, *Phys. Rev. B* **82**, 125444 (2010), doi:10.1103/PhysRevB.82.125444. IF 3.664, Cites **11**.

[35]"Gold and Methane: A Noble Combination for Delicate Oxidation", D. J. Mowbray, A. Migani, G. Walther, D. M. Cardamone, and A. Rubio, *J. Phys. Chem. Lett.* **4**, 3006 (2013), doi:10.1021/jz401553p, arXiv:1308.5266. IF 6.687, Cites **11**.

[36]"Quasiparticle spectra and excitons of organic molecules deposited on substrates: G_0W_0-BSE approach applied to benzene on graphene and metallic substrates", V. Despoja, I. Lončarić, D. J. Mowbray, and L. Marušić, Phys. Rev. B, 88, 235437 (2013), doi:10.1103/PhysRevB.88.235437 arXiv:1309.1359. IF 3.664, Cites **11**.

[37]"Channeling of protons through carbon nanotubes embedded in dielectric media", D. Borka, D. J. Mowbray, Z. L. Mišković, S. Petrovć, and N. Neškovć, *J. Phys.: Condens. Matter* **20**(47), 474212 (2008), doi:10.1088/0953-8984/20/47/474212. IF 2.223, Cites **10**.

[38]"The donut **a**nd dynamic polarization effects in proton channeling through carbon nanotubes", D. Borka, D. J. Mowbray, Z. L. Mišković, S. Petrović and N Nešković, *New J. Phys.*, **12**, 043021 (2010), doi:10.1088/1367-2630/12/4/043021 arXiv:1008.2629. IF 3.671, Cites **10**.

[39]"Calculation of the graphene C 1*s* core level binding energy", T. Susi, D. J. Mowbray, M. P. Ljungberg, and P. Ayala, *Phys. Rev. B* **91**, 081401(R) (2015), doi:10.1103/PhysRevB.91.081401 arXiv:1411.3874. IF 3.664, Cites 10 Rapid Communication.

[40]"A resonant photoemission insight into the electronic structure of Gd nanowires templated in the hollow core of SWCNTs", P. Ayala, R. Kitaura, C. Kramberger, H. Shiozawa, N. Imazu, K. Kobayashi, D. J. Mowbray, P. Hoffmann, H. Shinohara, and T. Pichler, *Materials Express*, **1**, 30 (2011), doi:10.1166/mex.2011.1004, Cites **8**.

[41]"Theoretical electron energy loss spectroscopy of isolated graphene", D. J. Mowbray *Phys. Status Solidi (b)*, **251**, 2509 (2014), doi:10.1002/pssb.201451174, arXiv:1408.6370. Cites **8**.

[42]"Computing C1s X-ray Absorption for Single-Walled Carbon Nanotubes with Distinct Electronic Type", D. J. Mowbray, P. Ayala, T. Pichler, and A. Rubio, *Materials Express* **1**, 225 (2011), doi:10.1166/mex.2011.1027. Cites **7**.

[43]"Using G_0W_0 Level Alignment to Identify Catechol's Structure on TiO_2(110)" D. J. Mowbray and A. Migani, *J. Phys. Chem. C*, **119**, 19634 (2015), doi:10.1021/acs.jpcc.5b05392, arXiv:1508.00786. IF 4.835 Cites **7**.

[44]"Influence of the dynamic polarization effect on the angular distributions of protons channeled in double-wall carbon nanotubes", D. Borka, S. Petrovć, N. Neškovć, D. J. Mowbray, and Z. L. Mišković, *Nucl. Instrum. & Methods Phys. Res. B* **256**, 131 (2007), doi:10.1016/j.nimb.2006.11.102. Cites **6**.

[45]"Channeling of charge carrier plasmons in carbon nanotubes", C. Kramberger, F. Roth, R. Schuster, R. Kraus, M. Knupfer, E. Einarsson, S. Maruyama, D. J. Mowbray, A. Rubio, and T. Pichler, *Phys. Rev. B* **85**, 085424 (2012), doi:10.1103/PhysRevB.85.085424. IF 3.664, Cites **5**.

[46]"Coverage Dependence of the Level Alignment for Methanol on TiO_2(110)", A. Migani and D. J. Mowbray, *Comput. Theor. Chem.* **1040-1041**, 259 (2014), doi:10.1016/j.comptc.2014.03.007, arXiv:1404.5154. Cites **5**.

[47]"Designing multifunctional chemical sensors using Ni and Cu doped carbon nanotubes", D. J. owbray, J. M. García-Lastra, K. S. Thygesen, A. Rubio, and K. W. Jacobsen, *Phys. Status Solidi (b)*, **247**, 2678 (2010), doi:10.1002/pssb.201000171. Cites 4.

[48]"Tuning MgB_2(0001) surface states through surface termination", V. Despoja, D. J. Mowbray, and V. M. Silkin, *Phys. Rev. B* **84**, 104514 (2011), doi:10.1103/PhysRevB.84.104514 arXiv:1105.2593. IF 3.664, Cites 4.

[49]"Modelling the effect of nuclear motion on the attosecond time-resolved photoelectron spectra of ethylene", A. Crawford-Uranga, U. De Giovannini, D. J. Mowbray, S. Kurth, and A. Rubio, *J. Phys. B – At. Mol. Opt. Phys.* **47**, 124018 (2014), doi:10.1088/0953-4075/47/12/124018 arXiv:1403.5408. Cites 4.

[50]"Using surface plasmonics to turn on fullerene's dark excitons", V. Despoja and D. J. Mowbray *Phys. Rev. B.* **89**, 195433 (2014), doi:10.1103/PhysRevB.89.195433, arXiv:1405.2860. IF 3.664, Cites 4.

[51]"PFO-BPy Solubilizers for SWNTs: Modelling Polymers from Oligomers", L. N. Glanzmann, D. J. Mowbray, and A. Rubio, *Phys. Status Solidi (b)*, **251**, 2407 (2014), doi:10.1002/pssb.201451171, arXiv:1411.3275. Cites 4.

List of Publications (continued)

[52]"Channeling of dipolar molecules through carbon nanotubes", D. J. Mowbray, S. Chung, Z. L. Mišković, and F. O. Goodman, *Nanotechnology* **18**, 424034 (2007), doi:10.1088/0957-4484/18/42/424034. IF 3.672, Cites 3.

[53]"Dynamic interactions of ions with carbon nanotubes in water", D. J. Mowbray, Z. L. Mišković, and F. O. Goodman, *Nucl. Instrum. & Methods Phys. Res. B* **256**, 167 (2007), doi:10.1016/j.nimb.2006.11.108. Cites 2.

[54]"Channeling of protons through carbon nanotubes", D. Borka, D. J. Mowbray, Z. L. Mišković, S.Petrovć, and N. Nešković, *J. Phys.: Conf. Ser.* **133**, 012015 (2008), doi:10.1088/1742-6596/133/1/012015. Cites 2.

[55]"Hydrodynamic modeling of fast ion interactions with carbon nanotubes", D. J. Mowbray, S. Chung, and Z. L. Mišković, in V. N. Popov and P. Lambin, eds., Carbon Nanotubes: From Basic Research to Nanotechnology (Springer, Dordrecht, 2006), pp. 176–177. Cites 1.

[56]"A combined photoemission and ab initio study of the electronic structure of (6,4)/(6,5) enriched single wall carbon nanotubes", K. De Blauwe, Y. Miyata, P. Ayala, H. Shiozawa, D. J. Mowbray, A. Rubio, P. Hoffmann, H. Kataura, and T. Pichler, *Phys. Status Solidi B* **247**, 2875 (2010), doi:10.1002/pssb.201000373. Cites 1.

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[61]"Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C_{60} and Polymer/SWNT Photovoltaic Devices", L. N. Glanzmann and D. J. Mowbray *J. Phys. Chem. C*, **120**, 6336 (2016) doi:10.1021/acs.jpcc.5b12611. IF 4.835.

[62]"Optical Absorption Spectra and Excitons of Dye-Substrate Interfaces: Catechol on TiO_2(110)", D. J. Mowbray and A. Migani *J. Chem. Theory Comput.* **12**, 2843 (2016) doi:10.1021/acs.jctc.6b00217. IF 5.310.

[63]"Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes", D. J. Mowbray, A. Pérez Paz, G. Ruiz-Soria, M. Sauer, P. Lacovig, M. Dalmiglio, S. Lizzit, K. Yanagi, A. Goldoni, P. Ayala, T. Pichler, and A. Rubio *J. Phys. Chem. C*, **120**, 18316 (2016) doi:10.1021/acs.jpcc.6b06163. IF 4.835.

Book Chapters

[1] L. Chiodo, J. M. García-Lastra, D. J. Mowbray, A. Iacomino, and A. Rubio, "Tailoring Electronic and Optical Properties of TiO_2: Nanostructuring, Doping and Molecular-Oxide Interactions", Ed. T. F. George, D. Jelski, R. R. Letfullin, and G. Zhang, in *Computational Studies of New Materials II: From Ultrafast Processes and Nanostructures to Optoelectronics, Energy Storage and Nanomedicine* World Scientific, Hackensack, NJ, Chapter 12, p. 301-330 (2011), doi:10.1142/9789814287197_0012 arXiv:1003.2341.

[2] D. J. Mowbray, J. M. García-Lastra, I. Larraza Arocena, Á. Rubio, K. S. Thygesen, K. W. Jacobsen, "Computational design of chemical nanosensors: Transition metal doped single-walled carbon nanotubes", Ed. G. Korotcenkov, in *Chemical Sensors: Simulation and Modeling Volume 2: Conductometric-Type Sensors*, Momentum Press, Highland Park, NJ, Chapter 9, (2012), doi:10.5643/9781606503140, arXiv:1112.1052.

[3] Y. Pouillon, A. Pérez Paz, J. Mäklin, N. Halonen, Y. Leroy, D. J. Mowbray, J. M. García Lastra, G. Tóth, K. Kordás, Z. Kónya, Á. Kukovecz, A. Rubio, "Gas Sensing and Thermal Transport Through Carbon-Nanotube-Based Nanodevices", in *Design and Applications of Nanomaterials for Devices and Sensors, Challenges and Advances in Computational Chemistry and Physics*, Ed. J. M. Seminario, Springer Vol. 16, Chapter 4, (2014), doi:10.1007/978-94-017-8848-9_4.

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Conferences

[1] *Ψ_k 2015* (Sep. 6 – Sep. 10 2015)
Poster presentations "*GW* and BSE at the Interface: The Role of Anisotropic Screening in Interfacial Level Alignment" and "Excitons in P3HT/SWNT/Fullerene heterojunctions" Ψ_k Conference, San Sebastián, Spain.

[2] *IWEPNM 2014* (Mar. 8 – Mar. 15 2014)
Poster Presentations "Using Theory to Deconvolute the XPS Spectra of Oxidized Metallicity-Sorted Carbon Nanotubes" and "Polymer-SWNT Hybrid Systems for Organic Solar Cells", International Workshop on Electronic Properties of Novel Materials 2011, Kirchberg, Austria.

[3] *APS March Meeting 2013* (Mar. 18 – Mar. 22 2013)
Oral Presentation "*GW* at the interface: CH_3OH and H_2O on TiO_2(110)", American Physical Society March Meeting 2013, Semiconductors: Theory and Spectra I, Baltimore, USA.

[4] *HPC-NN2011* (Apr. 14 2011)
Poster Presentation "Designing multifunctional chemical sensors using metal doped carbon nanotubes", High Performance Computing for Nanoscience & Nanotechnology 2011, Bilbao, Spain.

[5] *IWEPNM 2011* (Feb. 26 – Mar. 6 2011)
Poster Presentations "Using Theoretical Spectroscopy to Assess the Measured Electronic Structure of Doped Single Walled Carbon Nanotubes" and "Inspection of n and p-type substitutional dopants in SWCNTs and disentaglement of their bonding environment", International Workshop on Electronic Properties of Novel Materials 2011, Kirchberg, Austria.

[6] *MORE 2010* (Nov. 3 – Nov. 5 2010)
Oral Presentation "Calculating Electron Energy Loss Spectroscopy from First Principles", Meeting on Optical Response in Extended Systems 2010, Vienna, Austria.

[7] *Ψ_k 2010* (Sep. 12 – Sep. 16 2010)
Poster presentations "Designing multifunctional chemical sensors using metal doped carbon nanotubes", "Designing nanosensors using transition metal doped carbon nanotubes", and "Trends in metal oxide stability for nanorods, nanotubes, and surfaces", Ψ_k Conference, Berlin, Germany.

[8] *NDEEA10* (Apr. 26 – Apr. 27 2010)
Oral Presentation "Computational design of chemical nanosensors: Metal doped carbon nano-tubes", Nanoscale Devices for Environmental and Energy Applications, San Sebastián, Spain.

[9] *IWEPNM 2010* (Mar. 6 – Mar. 13 2010)
Poster Presentations "Computational design of chemical nanosensors: Metal doped carbon nanotubes", and "Optical Properties and Electronic Structure of (6,5) enriched SWCNT", International Workshop on Electronic Properties of Novel Materials 2010, Kirchberg, Austria.

[10]*Öresund Workshop* (Mar. 26 2009)
Oral Presentation "Using Carbon Nanotubes as Chemical Sensors", Öresund Workshop on Electron Transport in Nanostructures, Lund, Sweeden.

[11]*Nanotech North 2008* (Sep. 23 – Sep. 25 2008)
Oral Presentation "Influence of Physisorbed Molecules on Conductance of SWNT Networks: O_2 & N_2 Sensors", Nanotech Northern Europe 2008, Copenhagen, Denmark.

[12]*DCSC* (Apr. 1 2008)
Poster Presentation "Influence of Functional Groups on Charge Transport in Molecular Junctions", Danish Center for Scientific Computing, Kgs. Lyngby, Denmark.

[13]*NanoIP/PIC* (May 19 2006)
Poster Presentation "Hydrodynamic Modeling of Ion Storage in Carbon Nanotubes", 2006 Ontario Nano Symposium, Waterloo, Ontario, Canada.

[14]*Nano E / GDR-E05* (Oct. 10 – Oct. 13 2005)
Poster Presentation "Ion Interactions with Carbon Nanotubes in Dielectric Media", Science and Applications of Nanotubes, Houffalize, Belgium.

[15]*NATO Advanced Studies Institute* (May 21 – May 31 2005)
Oral Presentation "Hydrodynamic Modeling of Fast Ion Interactions with Carbon Nanotubes", Carbon Nanotubes: From Basic Research to Nanotechnology, Sozopol, Bulgaria.

[16]*International Centre for Theoretical Physics* (May 24 – Jun. 11 2004)
Poster Presentation "Ion Channeling Through Carbon Nanotubes", Spring College on Science at the Nanoscale, Trieste, Italy.

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Invited Talks

[1] "*GW* and BSE at the Interface: H_2O, CH_3OH, and Catechol on TiO_2"
(May 25, 2017) School of Physics Sciences and Engineering, Yachay Tech University, Urcuquí, Ecuador

[2] "The Role of Mathematical Modeling and Computer Simulation in Nanotechnology"
(Feb. 2, 2017) Depto. de Física de Materiales, Universidad del País Vasco UPV/EHU, Donostia, Spain.

[3] "The Role of Mathematical Modeling and Computer Simulation in Nanotechnology"
(Jul. 28 2016) Department of Applied Mathematics and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Canada.

[4] "The Role of Theory and Simulation in Nanotechnology Research"
(Jul. 7 2016) School of Physics Sciences and Engineering, Yachay Tech University, Urcuquí, Ecuador

[5] "GW and BSE at the Interface: H_2O, CH_3OH, and Catechol on TiO_2" *MANA-DIPC*
Nanostructures and Complex Functional Materials (Aug. 28 2015), DIPC, Donostia, Spain.

[6] "DFT Made Simple: Ground state properties of CNTs and molecules"
POCAONTAS Autumn School (Oct. 7 2014), Hotel Tivoli, Sintra, Portugal.

[7] "TDDFT Made Simple: Excited state properties of CNTs and molecules"
POCAONTAS Autumn School (Oct. 7 2014), Hotel Tivoli, Sintra, Portugal.

[8] "Theoretical Spectroscopy of Graphene and Carbon Nanotubes",
(Jun. 12 2012) Department of Physics & Institute of Physics, University of Zagreb, Zagreb, Croatia.

[9] "Theoretical Spectroscopy of Graphene and Carbon Nanotubes",
(Oct. 4 2012) Department of Applied Mathematics, University of Waterloo, Waterloo, Canada.

[10]"Catalysis by Gold",
(Jun. 7 2012) Institute of Computacional Chemistry, University of Girona, Girona, Spain.

[11]"Carbon Nanotube Based Chemical Sensors: A Computational Design Approach",
(Jan. 5 2012) Department of Applied Mathematics, University of Waterloo, Waterloo, Canada.

[12]*Theory Days on Q dots & wires* (Nov. 17 – Nov. 19 2010)
"Carbon Nanotube Based Chemical Sensors: A Computational Design Approach",
Theory Days on Quantum Dots and Wires, Toulouse, France.

[13]"Designing Carbon Nanotube Based Chemical Sensors"
(Nov. 12 2009) Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.

[14]"Three Major Challenges for the Computational Design of Nanoelectronics and Nanosensors",
(Dec. 15 2008) Department of Applied Mathematics, University of Waterloo, Waterloo, Canada.

Grants & Projects

POCAONTAS	POlymer / CArbOn NanoTubes Active Systems	FP7-2012-316633	237,296 €	2012–2016
DYNAPLEX	Dynamical processes in complex quantum systems: from theoretical developments to energy harvesting and storage	FIS2010-21282C0201	213,565 €	2012
consolider nanoTHERM	Tailoring electronic and phononic properties of nanomaterials: Towards ideal Thermoelectricity	CSD2010-00044	385,000 €	2011–2015
ICC	International Collaboration in Chemistry: Molecules at Nanostructured Surfaces for Solar Cell Applications	PIB2010US-00652	210,500 €	2010–2013
ACI-promociona	Desarrolo de la Vicepresidencia Cientifíca de la ETSF	ACI2009-1036	108,000 €	2009–2012
e-I3-ETSF	European Theoretical Spectroscopy Facility	INFRA2007-211956	495,835 €	2008–2011

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Supervisor for European Theoretical Spectroscopy Facility User & Training Projects

#337	"Electronic structure of (6,4) and (6,5) single wall carbon nanotubes"	Prof. T. Pichler	Jun. 2010
#338	"Raman spectroscopy of single walled, double walled, and bundled carbon nanotubes"	Prof. H. Kuzmany	Jun. 2010
#381	"Engineering photodissociation states in polyaromatic halides	Dr. C. A. Palma	Dec. 2010
#391	"Anisotropy in the loss-function of potassium intercalated single wall carbon nanotube bundles"	Dr. C. Kramberger	Jul. 2011

References

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