List of Publications – Dr. Duncan John Mowbray

List of Publications (ordered by number of citations)

[1] "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 **117**.

[2] "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 **111**.

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[41]"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 **5**.

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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 in press* (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.

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List of Publications – Dr. Duncan John Mowbray

List of Publications (Corrections and Erratums)

[1] Correction to "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*, **120**, 4151 (2016), doi:10.1021/acs.jpcc.6b01244. IF 4.835 Cites 1.

[2] Publisher's Note: Plasmon excitations on a single-wall carbon nanotube by external charges: Two-dimensional two-fluid hydrodynamic model [Phys. Rev. B **82**, 035405 (2010)] D. J. Mowbray, S. Segui, J. Gervasoni, Z. L. Mišković, and N. R. Arista, *Phys. Rev. B* **82**, 119903 (2010), doi:10.1103/PhysRevB.82.119903. IF 3.664.