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DANIEL GONZÁLEZ TRABADA First-principles Atomistic Simulation Techniques

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Biographical Info

2010 Máster Universitario en Formación del Profesorado de ESO y Bachillerato, FP y Enseñanzas de Idiomas.

2009 PhD at the UAM.

2005 Physics degree at the UAM.

Honors and Awards

Research Interests

First-principles Molecular Dynamics.

Simulation of reactions in biomolecules.

Dynamical, atomic and electronic properties of semiconductor surface.

Relevant/Recent Publications

Quantum Mechanics/Molecular Mechanics Free Energy Maps and Nonadiabatic Simulations for a Photochemical Reaction in DNA: Cyclobutane Thymine Dimer, Jesús I. Mendieta-Moreno, Daniel G. Trabada, Jesús Mendieta, James P. Lewis, Paulino Gómez-Puertas, and José Ortega, J. Phys. Chem. Lett., 7 (21), pp 4391–4397, (2016). [URL]

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Ibrahimi, D. G. Trabada, J. Ortega, and F. Flores, Phys. Rev. Lett. 107, 187603, (2011). [URL]
Advances and applications in the FIREBALLab initio tight-binding molecular-dynamics formalism, Lewis, J. P., Jelínek, P., Ortega, J., Demkov, A. A., Trabada, D. G., Haycock, B., Wang, H., Adams, G., Tomfohr, J. K., Abad, E., Wang, H. and Drabold, D. A., Phys. Status Solidi B, 248: 1989–2007, (2011). [URL]
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Weak dimers and soft phonons on the β-SiC(100) surface, Daniel G Trabada and José Ortega, Journal of Physics: Condensed Matter, 21(18), (2009). [URL]