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Biographical Info

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Research Interests

First-principles Molecular Dynamics.

Simulation of reactions in biomolecules.

Dynamical, atomic and electronic properties of semiconductor surfaces.

Organic Interfaces.

Nanocontacts, nanowires and nanotubes.

Relevant/Recent Publications

Nonadiabatic ensemble simulations of cis-Stilbene and cis-Azobenzene

Photoisomerization. A.J. Neukirch, L.C. Shamberger, E. Abad, B.J. Haycock, Hong Wang, J. Ortega O.V. Prezhdo and J.P. Lewis, JOURNAL OF CHEMICAL THEORY AND COMPUTATION 10, 14 (2014). [\[URL\]](#)

Calculation of non-adiabatic coupling vectors in a local-orbital basis set. E. Abad, J.P. Lewis, V. Zobac, P. Hapala, P. Jelínek and J. Ortega. THE JOURNAL OF CHEMICAL PHYSICS 138, 154106 (2013). [\[URL\]](#)

Energy level alignment in Organic-Organic heterojunctions: the TTF/TCNQ interface. J.I. Beltrán, F. Flores, J.I. Martínez and J. Ortega. THE JOURNAL OF PHYSICAL CHEMISTRY C 117, 3888 (2013). [\[URL\]](#)

Improvement of Scanning Tunneling Microscopy Resolution with H-Sensitized Tips. J.I. Martínez, E. Abad, C. González, F. Flores and J. Ortega. PHYSICAL REVIEW LETTERS

108, 246102 (2012). [\[URL\]](#)

Giant alkali-induced lattice relaxation as the driving force of the insulating phase of alkali/Si(111):B L. Chaput, C. Tournier-Colletta, L.A. Cardenas, A. Tejada, B. Kierren, D. Malterre and Y. Fagot-Revurat, P. Le Fevre, F. Bertran and A. Taleb-Ibrahimi, D.G. Trabada, J. Ortega and F. Flores. PHYSICAL REVIEW LETTERS 107, 187603 (2011).

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Initial Stages of the Contact between a Metallic Tip and Carbon Nanotubes. C. González, J. Ortega, F. Flores, D. Martínez-Martín and J. Gómez-Herrero. PHYSICAL REVIEW LETTERS 102, 106801 (2009). [\[URL\]](#)

Mechanism of Band Gap Opening across the Order-Disorder Transition of Si(111)4×1-In. C. González, J.D. Guo, J. Ortega, F. Flores and H.H. Weitering. PHYSICAL REVIEW LETTERS 102, 115501 (2009). [\[URL\]](#)

Hydrogenation of semiconductor interfaces: Si-terminated cubic SiC(100) surfaces. D.G. Trabada, F. Flores and J. Ortega. PHYSICAL REVIEW B 80, 075307 (2009). [\[URL\]](#)

Fullerenes from aromatic precursors by surface-catalysed cyclodehydrogenation. G. Otero, G. Biddau, C. Sánchez-Sánchez, R. Caillard, M.F. López, C. Rogero, F.J. Palomares, N. Ca bello, M.A. Basanta, J. Ortega, J. Mendez, A.M. Echavarren, R. Pérez, B. Gómez-Lor, J.A. Martín-Gago. NATURE 454, 865-868 (2008). [\[URL\]](#)

Barrier formation at organic interfaces in a Cu(100)-benzenethiolate-pentacene heterostructure. M.G. Betti, A. Kanjilal, C. Mariani, H. Vázquez, Y.J. Dappe, J. Ortega and F. Flores. PHYSICAL REVIEW LETTERS 100, 027601 (2008). [\[URL\]](#)

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