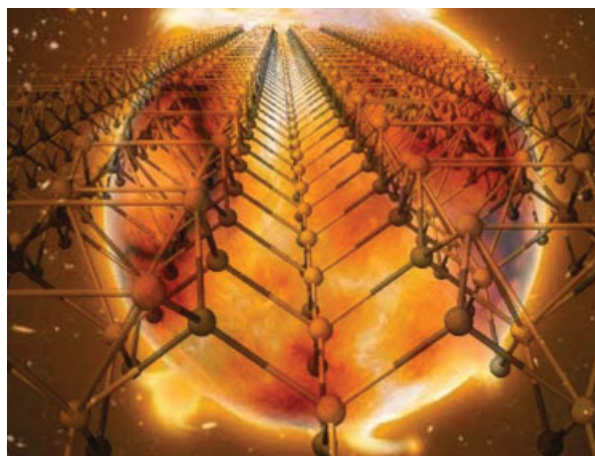


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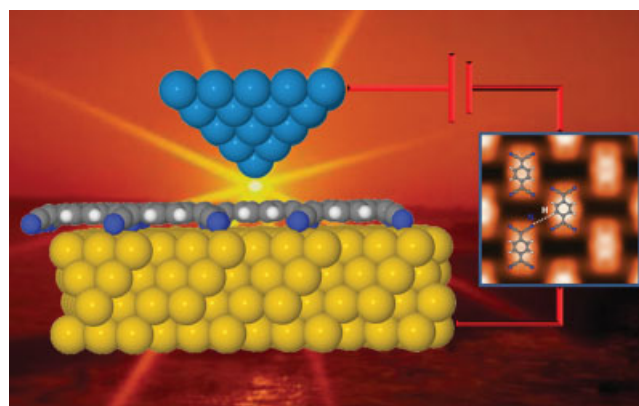
FRONT COVER



The front cover image of this issue shows the “Fireball” – an artistic ball and stick view (by Daniel G. Trabada) of the β -SiC(100) surface. The background alludes to the first-principles molecular-dynamics technique FIREBALL (see the Review Article by James P. Lewis et al. on pp.1989–2007): The “fireball” orbitals used in this computational approach are obtained from atomic calculations in which the orbitals are confined within a given cut-off radius. The effect of this confinement is to increase the energy of the atoms, depicted here as microscopic “balls of fire”. The FIREBALL method is based on the Sankey–Niklewski approach, one of the outstanding advancements in electronic structure density-functional methods. Lewis et al. report on several improved theoretical developments and recent application to a variety of systems ranging from biomolecules to semiconductors. The review and 12 more articles in this issue compose the special section “Large-scale simulations in materials science”, dedicated to Otto F. Sankey (see pp. 1987–1988).

BACK COVER

The growing market of organic electronics relies on the use of organic conjugated molecules as components of multilayer devices, whose performance depends critically on the energy barriers that control the carrier transport between layers, and the electronic transport in a nanocontact between a single molecule and metal electrodes. As shown by José I. Martínez et al. (pp. 2044–2049), theoretical STM imaging arises as a powerful tool in this novel researching field, validating the obtained interfacial geometries compared with the experimental STM for the TCNQ/Au(111) self-assembled structure, as well as the complementary electronic structure analysis.



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➤ ORIGINAL PAPERS

Large-scale simulations in materials science

Guest Editors: David Drabold, Alex Demkov, James P. Lewis, José Ortega, Wolfgang Windl, and Stuart Lindsay

Page 1987–1988	Dedication to Otto F. Sankey
Page 1989–2007	Review Article James P. Lewis, Pavel Jelínek, José Ortega, Alexander A. Demkov, Daniel G. Trabada, Barry Haycock, Hao Wang, Gary Adams, John K. Tomfohr, Enrique Abad, Hong Wang, and David A. Drabold Advances and applications in the FIREBALL <i>ab initio</i> tight-binding molecular-dynamics formalism
Page 2008–2014	Feature Article Chen-Wei Jiang, Xiang Zhou, Zhibin Lin, Rui-Hua Xie, Fu-Li Li, Meng Gao, and Roland E. Allen Semiclassical simulations in materials science
Page 2015–2026	Feature Article MingLiang Zhang and D. A. Drabold The microscopic response method: Theory of transport for systems with both topological and thermal disorder
Page 2027–2031	Ting Luo, Caixia Zhang, Zhiyong Zhang, Yingdan Zhu, and Jun Li Rational designs of crystal solid-solution materials for lithium-ion batteries
Page 2032–2036	Antonis N. Andriotis and Madhu Menon Magnetic coupling in dilute magnetic semiconductors: A new perspective
Page 2037–2043	Hong Wang and James P. Lewis The reactive sites in faceted anatase nanoparticles
Page 2044–2049	José I. Martínez, Enrique Abad, Fernando Flores, and José Ortega Simulating the organic-molecule/metal interface TCNQ/Au(111)
Page 2050–2055	Yaojun A. Du, Thomas J. Lenosky, Richard G. Hennig, Stefan Goedecker, and John W. Wilkins Energy landscape of silicon tetra-interstitials using an optimized classical potential
Page 2056–2063	Mohammad Sherafati and Sashi Satpathy Impurity states on the honeycomb and the triangular lattices using the Green's function method
Page 2064–2071	Xiang Chen and John C. H. Spence On the measurement of the Casimir torque
Page 2072–2075	Barry Haycock, José Ortega, and James P. Lewis Failure of potassium dimer formation on the β-SiC(100)-c(4×2) surface

- Page **2076–2081** _____ A. A. Demkov, A. Posadas, H. Seo, J. K. Lee, and N. Sai
Emerging physics of oxide heterostructures
- Page **2082–2086** _____ Y. Li, F. Inam, Avishek Kumar, M. F. Thorpe, and D. A. Drabold
Pentagonal puckering in a sheet of amorphous graphene

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➤ ORIGINAL PAPERS

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