

Journal of Physics

Condensed Matter

Volume 25 Number 47 27 November 2013

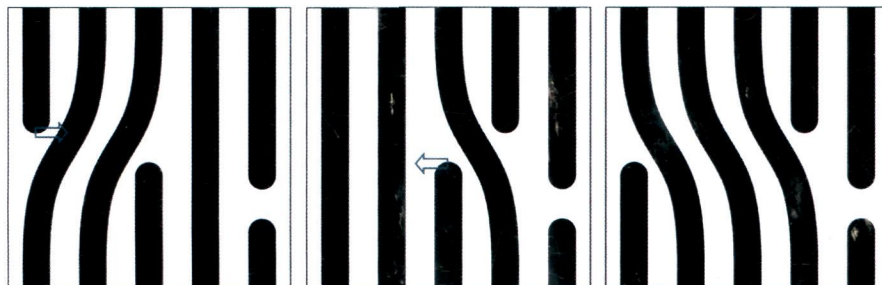
Topical reviews

Quantifying charge transfer energies at donor–acceptor interfaces in small-molecule solar cells with constrained DFTB and spectroscopic methods

Reinhard Scholz, Regina Luschnitz, Gotthard Seifert, Till Jägerle-Hoheisel, Christian Körner, Karl Leo and Mathias Rapacioli

Pseudopotential-based studies of electron transport in graphene and graphene nanoribbons

Massimo V Fischetti, Jiseok Kim, Sudarshan Narayanan, Zhun-Yong Ong, Catherine Sachs, David K Ferry and Shela J Aboud



FAST TRACK COMMUNICATIONS

- 472201 **Thin film MnGe grown on Si(111)**
J Engelke, D Menzel and V A Dyadkin
- 472202 **Impact of Joule heating, roughness, and contaminants on the relative hardness of polycrystalline gold**
Christopher R Freeze, Xiaoyin Ji, Angus I Kingon and Douglas L Irving
- 472203 **Graphene mediated domain formation in exchange coupled graphene/Co₃O₄(111)/Co(0001) trilayers**
Yi Wang, Lingmei Kong, Frank L Pasquale, Yuan Cao, Bin Dong, Iori Tanabe, Christian Binek, Peter A Dowben and Jeffry A Kelber

TOPICAL REVIEWS

- 473201 **Quantifying charge transfer energies at donor–acceptor interfaces in small-molecule solar cells with constrained DFTB and spectroscopic methods**
Reinhard Scholz, Regina Luschinetz, Gotthard Seifert, Till Jägeler-Hoheisel, Christian Körner, Karl Leo and Mathias Rapacioli
- 473202 **Pseudopotential-based studies of electron transport in graphene and graphene nanoribbons**
Massimo V Fischetti, Jiseok Kim, Sudarshan Narayanan, Zhun-Yong Ong, Catherine Sachs, David K Ferry and Shela J Aboud

PAPERS

NANOSTRUCTURES AND NANOELECTRONICS

- 475301 **Estimating the elastic properties of few-layer graphene from the free-standing indentation response**
Lixin Zhou, Yugang Wang and Guoxin Cao
- 475302 **Stability of the Tomonaga–Luttinger liquid state in gamma-irradiated carbon nanotube bundles**
B A Danilchenko, N A Tripachko, E A Voitsihovska, I I Yaskovets, I Y Uvarova and B Sundqvist
- 475303 **Boundary condition and pre-strain effects on the free standing indentation response of graphene monolayer**
Lixin Zhou, Yugang Wang and Guoxin Cao
- 475304 **Probing Majorana modes in the tunneling spectra of a resonant level**
R Korytár and P Schmitteckert

SOLID STRUCTURE AND LATTICE DYNAMICS

- 475401 **Charge carriers and small-polaron migration as the origin of intrinsic dielectric anomalies in multiferroic TbMnO₃ polycrystals**
L G D Silveira, G S Dias, L F Cótica, J A Eiras, D Garcia, J A Sampaio, F Yokaichiya and I A Santos
- 475402 **Structural study of α -Bi₂O₃ under pressure**
A L J Pereira, D Errandonea, A Beltrán, L Gracia, O Gomis, J A Sans, B García-Domene, A Miquel-Veyrat, F J Manjón, A Muñoz and C Popescu
- 475403 **Study of crystal-field excitations and infrared active phonons in the multiferroic hexagonal DyMnO₃**
S Jandl, S Mansouri, J Vermette, A A Mukhin, V Yu Ivanov, A Balbashov and M Orlita
- 475404 **Molecular dynamics evidence for alkali-metal rattling in the β -pyrochlores, AO₂O₆ (A = K, Rb, Cs)**
E Shoko, V K Peterson and G J Kearley

ELECTRONIC STRUCTURE

- 475501 **Effect of doping on electronic structure and photocatalytic behavior of amorphous TiO₂**
Kulbir Kaur Ghuman and Chandra Veer Singh

(Continued on inside back cover)

- 475502 Prediction of a large number of electron pockets near the band edges in type-VIII clathrate Si₄₆ and its physical properties from first principles**
Payam Norouzzadeh, Charles W Myles and Daryoosh Vashaee
- SUPERCONDUCTORS AND METALS
- 475701 Superconducting pairing and the pseudogap in the nematic dynamical stripe phase of La_{2-x}Sr_xCuO₄**
S Sugai, Y Takayanagi, N Hayamizu, T Muroi, R Shiozaki, J Nohara, K Takenaka and K Okazaki
- SEMICONDUCTORS
- 475801 Origin of n- and p-type conductivity in undoped α -PbO: role of defects**
J Berashevich, J A Rowlands and A Reznik
- DIELECTRICS AND FERROELECTRICS
- 475901 Atomic distribution, local structure and cation size effect in o-R_{1-x}Ca_xMnO₃ (R = Dy, Y, and Ho)**
Ning Jiang, X Zhang and Yi Yu
- MAGNETISM AND MAGNETIC MATERIALS
- 476001 Manifestation of long-range ordered state in layered VX₂ (X = Cl, Br, I) systems**
A H M Abdul Wasey, Debjani Karmakar and G P Das
- 476002 Direct evidence for nuclear spin waves in Nd₂CuO₄ by high-resolution neutron-spin-echo spectroscopy**
Tapan Chatterji, Olaf Holderer and Harald Schneider
- 476003 Magnetic properties of ultrathin Ni₈₁Fe₁₉ films with Ta and Ru capping layers**
S Kezilebieke, M Ali, B Shadeke and R Gunnella