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Investigation of the $CuIn_{1-x}Al_xSe_2$ structure-properties relationships by coupling density functional and Bader's theories

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For three decades density functional theory (DFT) has imposed itself as an accurate quantum method to investigate materials properties. In parallel, developments of density based descriptors such as Bader's quantum theory of atoms in molecules (QTAIM) brought new insights into the chemical bonding of materials. The ternary Cu-based chalcopyrite compound, $CuInSe_2$ (CIS), is an interesting material as solar cell absorber layer due to its low cost, high absorption coefficient, excellent optical and electrical properties. Many approaches have been adopted to improve its energy conversion efficiency. However, its narrow band gap and the scarcity and expensiveness of indium constrain its large-scale development. Replacing indium by the abundant and inexpensive aluminum to form the quaternary $CuIn_{1-x}Al_xSe_2$ (CIAS), has been considered as a promising alternative with few changes in physical and chemical properties. In this work, we investigated by DFT calculations the structural, electronic and optical properties of $CuIn_{1-x}Al_xSe_2$, for various "x" from 0 to 1, and determined the optimal substituting percentage. Moreover, in current PV cells, strains originating from the lattice mismatch between the PV materials and the substrates inevitably influence the optical performances, we calculated the band gap and optical properties for the optimal alloy subjected to biaxial strains. In the aim to unravel the deep relationship between bond interactions and optical properties, a detailed investigation of topological properties based on the electron density has been conducted as strain is applied.

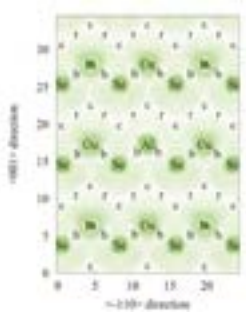

Figure: Electron density map with bond (b) critical points (CP) ring (r) CP and cage (c) CP.

Recent Publications

1. H J Meadows, S Misra, B J Simonds, M Kurihara, T Schuler, V Reis-Adonis, A Bhatia, M A Scarpulla and P J Dale (2017) Journal of Materials Chemistry C 5:1336–1345.
2. O Meglali, A Bouraiou, N Attaf and M S Aida (2017) Optik - International Journal for Light and Electron Optics 140:709–717.
3. K C Huang, C L Liu, P K Hung and M P Houng (2013) Applied Surface Science 273:723–729.

4. W Deng, Z Yan, Y Fang and Y Wang (2014) Journal of Materials Science: Materials in Electronics 25: 2829–2834.
5. J López-García and C Guillén (2009) Thin Solid Films 517:2240–2243.
6. K W Cheng, K Hinaro and M P Antony (2016) Solar Energy Materials and Solar Cells 151:120–130.

Biography

Marie-Christine Record is Full Professor of Materials Chemistry at the University of Aix-Marseille, France since 2004. Her field of interest is solid state chemistry both from the experimental and computational stand points. Her experimental skills spread from the determination of phase diagrams and the synthesis of materials, by using methods as varied as mechanical alloying, self-propagating high temperature synthesis (SHS), reactive diffusion in thin films and electro chemical atomic layer epitaxy (EC-ALD), to materials structures (X-ray diffraction) and properties (electronic) characterization. For the purpose of better understanding the materials structure-properties relationships, she has developed for more than a decade computational strategies based on ab initio methods. She has been working on different kinds of materials such as intermetallics, chalcogenides for application purposes, especially for thermoelectric ones. She is author and co-author of more than 90 papers published in international scientific journals.

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