nitrogen, oxygen, boron, alkali metals, calcium, $CaCO_3$ and $MgCO_3$, CO_2 and CH_4 - [1,3-9]), some of which will be presented in this talk.
〔1〕 Oganov A.R. & Glass C.W. (2006). *J. Chem. Phys* **124**, art. 244704.
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Keywords: high pressure, phase transitions, density functional theory

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Theoretical prediction and characterization of high pressure structures and properties of calcium

Dennis D Klug[1], Yansun Yao[2], John S Tse[2], Jian Sun[1], Yvon Le Page[3]
[1]National Research Council of Canada, Steacie Inst. for Molecular Sciences, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6, Canada, [2]Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, Saskatchewan, Canada, S7N 5E2, [3]ICPET, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6, E-mail：Dennis.Klug@nrc.ca

This study employed a combination of theoretical techniques to predict the structure and properties of calcium IV and V at high pressures. Structural predictions for calcium in the pressure range 120－160 GPa were obtained with a genetic algorithm and with a pseudo-random search method. The X-ray diffraction pattern of the resulting structures are in excellent agreement with recent experimental results. Phonon and electron-phonon calculations were performed with plane-wave density functional methods to investigate the stabilities and potential superconductivity. The proposed structures are both found to be superconducting and the calculated Tc values are close to those observed for Ca-IV and V. Theory indicates a superconducting transition at 25 K for the structures obtained in this study, in excellent agreement with experiment. Analysis of a recent theoretically predicted structure indicates that this structure may be unstable at high pressures

Keywords: *ab initio* calculations, calcium, high pressure studies

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Polymorphism and structural phase transitions in crystals: Computer simulations by metadynamics

Roman Martonak
Faculty of Mathematics, Physics and Informatics, Comenius University, Department of Experimental Physics, Mlynska dolina F2, Bratislava, Bratislava, 842 48, Slovak Republic, E-mail：martonak@fmph.uniba.sk

The talk will present the recently developed algorithm for simulation of structural phase transitions in crystals[1,2]. The new approach is based on the general metadynamics algorithm[3] and searches for low-energy pathways leading from one crystal structure to another. It enables also simulation of complex reconstructive transitions with transformation pathways proceeding via several intermediate states, resulting in substantially improved predictive power. The applications of the algorithm will be demonstrated on several systems, with focus on silica[4] and carbon dioxide. We performed an extensive study aimed at investigation of structural transformations in silica and demonstrated that starting from α-quartz it is possible to find nearly all silica polymorphs observed in the range of pressures from zero to several Mbar. We also investigate pressure-induced phase transitions of α-cristobalite [5]. In carbon dioxide we study the interesting mechanisms of transformation of molecular phases to polymeric phases at high pressure. The results demonstrate that the new method is far more efficient than previous ones and for the first time the study of complex structural transformations with many intermediates is within the reach of molecular dynamics (MD) simulations.
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First-principles calculations of pressure induced magnetic transition in siderite $FeCO_3$

Wei Luo[1,2], Hongting Shi[2], Rajeev Ahuja[1,2]
[1]Uppsala University, Condensed Matter Theory Group, BOX 530, Uppsala, Uppsala, SE-751 21, Sweden, [2]Condensed Matter Theory Group, Uppsala University, BOX 530, Uppsala SE-751 21, Sweden, E-mail：wei.luo@fysik.uu.se

Rhombohedral siderite $FeCO_3$ has been studied by using density functional theory (DFT) with the generalized gradient approximation (GGA). In order to take into account the strong on-site Coulomb interaction U present in $FeCO_3$, we also performed the GGA + U calculations. We observed a pressure-induced magnetic transition (high spin -> low spin) at pressures of 15 GPa and 28 GPa, which were underesimated with respective to the experiment, for the GGA and GGA + U calculations, respectively. This phase transition was with a volume collapse of 10% around, also accompanied by an