Poster Sessions

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Surface modification of hydroxyapatite by grafting alkyl phosphonic dichloride

Hassen Agougui, Abdallah Aissa, Mongi D debbbi, Laboratoire de Physico-Chimie des Matériaux, Faculté des Sciences de Monastir, 5019 Monastir, (Tunisia). E-mail: Hassenagougui@yahoo.fr

The inorganic-organic hybrids have interesting applications resulting from the combination of some characteristic properties of the inorganic substrate (mechanical and chemical properties, exchange capacity, bioreactivity, optical properties...) with those of the organic grafting (polymerizability, superficial tension...). Such modified materials are used in catalysis, chromatography, biomedical domain...

We have computed the elastic stiffness tensors of ZrO2 and HfO2 polymorphs with baddeleyite-type (P21c), Pbca and cotunnite-type (Pnma) structures in order to obtain the anisotropy of sound wave phase velocities and have calculated the thermodynamic mixing properties of HfO-ZrO2 solid solutions with the cotunnite structure. The calculations were based on density functional theory within the generalized gradient approximation (GGA) with PBE and PBEsol functionals [5, 6]. The calculations were carried out with the program CASTEP [7] using high-performance computers at the University of Frankfurt and at the Moscow State University.

The anisotropic sound wave phase velocities were determined using the Christoforff tensor [8]. Despite the lower stiffness, the calculated speeds of sound wave propagation are generally higher for ZrO2 polymorphs because of their lower density.

Keywords: solid_solution, elastic_property

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An ab initio study of ZrO2-HO2 solid solution with cotunnite structure

Alexandra M. Goryaeva, Victor L. Vinograd, Bjorn Winkler, Nikolay N. Eremin, Vadim S. Usurov, Institute of Crystallography and Crystal Chemistry, Moscow State University, Moscow (Russia). Institute of Energy and Climate Research (IEF-6), Forschungszentrum Jülich, Jülich (Germany). Institute of Geosciences, University of Frankfurt, Frankfurt a.M. (Germany). E-mail: a.goryaeva@mail.ru

Previous experimental and theoretical studies [1], [2], [3], [4] suggested that cotunnite-type zirconia and hafnia, as well as their solid solutions, could be candidates for superhard materials due to their high bulk moduli. Another possible application of cotunnite-type ZrO2 and HfO2 as waveguide materials is discussed here. An investigation of these questions requires knowledge of the elastic stiffness tensor as a function of chemical composition. According to the results of ab initio calculations [2, 4 and this study] the elastic stiffness coefficients of the HfO2 polymorphs are significantly larger than those of the corresponding ZrO2 polymorphs, while the volumes of the ZrO2 polymorphs are consistently smaller. It is not obvious whether the contraction of the HfO2 structure due to the incorporation of a smaller, but more compressible cation causes an increase in the bulk modulus, or how the incorporation of the larger, but less compressible Hf cation changes the elastic stiffness properties of ZrO2.

Keywords: framework, expansion, cyanide

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Crystal structures and ultramicroporosity in Mg & Ca tetraphosphate hydrates

Rosario M. Pérez Colodrero, Aurelio Cabeza Díaz, Jordi Rius, Pascual Olivera-Pastor, Konstantinos D Demadis, Didier Villemin, Miguel Angel Garcia Aranda, Departamento de Química Inorgánica, Universidad de Málaga, Malaga (Spain), Institut de Ciencies de Materials de Barcelona, Bellaterra, Catalunya (Spain).

Crystal Engineering, Growth & Design Laboratory, Department of Chemistry, University of Crete, Heraklion, Crete (Greece). UMR CNRS 6597, INCM3, Université de Caen, Caen (France). E-mail: colodrero@uma.es

The chemistry of hybrid organic-inorganic materials has experimented, during the past decade, an exponential growth due to the high number of possible applications in many fields such as gas storage, catalysis, and ion exchange [1]. The phosphate-based metal organic framework are today under investigation, and it is a common opinion that the best results are forthcoming. This is mainly due to the fact that generally the phosphonic acids have a higher flexibility degree, with respect to the carboxylic ligands, leading to a major structural variability and therefore to a lower control in their design.

Keywords: solid_solution, elastic_property