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Characterization of the electronic structures and properties of lithium silicates crystals and glasses

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Lithium silicates play an important role in, for example, the ceramics industry, in electronics and photonic devices, and in nuclear waste immobilization. The characterization of atomic and electronic properties are, therefore, important to optimize the fabrication and operation of lithium silicate containing materials. Density functional theory calculations within the generalized gradient approximation were employed to study the structure, dynamics, and electronic properties of lithium silicate crystals and glasses. The consistency and inconsistencies of crystal structure with respect to experiment will be presented. An emphasis of this work is in the use of Bader and Hirshfeld analysis used to capture the effective or relative charge differences based on using the electron density. It is found that the underlying difference in the methods is partly due to how the charge density is partitioned, where an alternative Bader analysis is used to reveal this difference. Atomic charge analysus are used to obtain the relative ionicity where the results are compared to chemical intuition as a means to consolidate them. Glass structures were generated using molecular dynamics simulations and where the diffusion mechanisms of the ions are obtained for the melt phases. The electron density of states for the glass and crystal systems was obtained and compared with one another where marked differences are observed and related to the crystal versus amorphous structures.

Jeudi 9 novembre 2006 à 10h30

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