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First principle computational modeling of electronic and structural properties of zeolites by using periodic DFT

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Zeolites are microporous, crystalline, hydrated aluminosilicate minerals known for their function as "molecular sieves." They are widely used for ion exchange, adsorption, and catalysis. In the present study, the main focus was on calculating electronic and structural properties of zeolite frameworks using periodic DFT. The unit cells of LTA, FAU, MER, and CHA type zeolites were used, and all the calculations were performed by using the Quantum ESPRESSO software package. To obtain a structure consistent with the DFT-PBE functional, all the frameworks of unit cells were relaxed by doing full variable relaxation (vc-relax) calculations. The plane-wave kinetic energy cutoff (ecutwfc) and the k-point grid sampling of the Brillouin zone were converged, exchange-correlation interactions were treated within the generalized gradient approximation (GGA) using the Perdew-Burke Ernzerhof (PBE) functional. Electron-ion interactions were described using pseudopotentials that were taken from the Quantum Espresso pseudopotential library. To obtain the electronic density of state (DOS) and band structure with high resolution, a non-self-consistent field (NSCF) calculation was performed. Phonon calculations were performed on the LTA zeolite to determine the theoretical IR vibrational modes. Optimized Si-O bond lengths were located in 1.60 Å – 1.62 Å range, Si-O-Si bond angles ranged from 149^0 to 151^0, The band gap values of LTA, FAU, MER and CHA zeolite types are 5.48 eV, 5.56 eV, 5.64 eV and 5.92 eV respectively. The Si-O-Al symmetric vibrations appeared at 665 cm^{-1}, Si-O-Si asymmetric vibrations were located at 926 cm^{-1}. The theoretical and experimental unit-cell dimensions, band gaps, are located within the acceptable range. Theoretical IR vibrational frequencies were in agreement with experimental values. These findings confirm that integration of periodic DFT calculations adds a powerful theoretical dimension to the study of properties of zeolite frameworks.

Keywords:

Zeolite, Electronic structure, Structural properties, Density functional theory (DFT), Quantum ESPRESSO