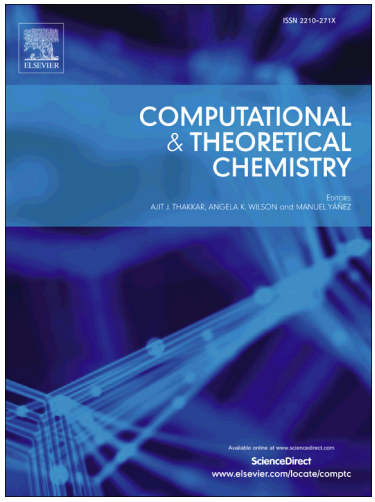

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Evolution of the structural and electronic properties of small alkali metal-doped aluminum clusters

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Abstract

The atomic arrangement of Al_n and Al_nM clusters (n = 2 - 14, M = Li, Na o K) was determined by combining both the basin hopping (BH) algorithm using the Gupta potential, and density functional theory (DFT) calculations. The BH yielded hundreds of structures that were refined by DFT using the PBE framework, and Ahlrichs-VDZ basis sets. Anions, neutrals and cations of Al_n and Al_nM clusters were calculated by DFT resulting in a set of ground state structures. These structures were considered for studying different stability criteria such as binding energy,