Density functional studies of protonated and alkali metal (Li, Na and K) incorporated T-doped 2D zeolite model (T= B, Ga)

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Density functional theory (DFT) method as implemented in the Quantum Espresso packages was used to investigate the effects of trivalent atoms such as B and Ga substituting Si atom in a bilayer silica material. This bilayer system was recently proposed by researchers from Brookhaven lab (Boscoboinik et *al.* [1]) as a suitable candidate for 2D representative of zeolites. The effects of the trivalent atoms on the stability, structural and electronic properties of the 2D zeolite model were explored. The formation energy analysis revealed that the introduction of B atom is exothermic whereas that of Ga atom is endothermic. Next, the introduction of B and Ga were found to affect the bond lengths of the system, however, it does not lead to a significant deformation of the structure. Regarding the electronic properties, the Fermi level was shifted towards the valence band revealing the obtention of p−type materials. The presence of B and Ga atoms in bilayer material results in a net negative charge to the framework. In the present study, proton and alkali metals were considered as charge balance. Their suitable site preference as well as the best candidate for charge balance were identified. The density of states analysis showed that the presence of cations induces defect states near the band edges narrowing the band gap. Our results provide detailed information about the properties of the doped silica bilayer at the atomic level which is beneficial for its nanotechnological applications as well as for its fully validation as 2D model for zeolite.

[1] Boscoboinik, J. Anibal, and Shamil Shaikhutdinov. *Catalysis letters* 144.12 (2014): 1987-1995.