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Table 7.5 The binding energies, substitutional energies and magnetic moments of Mg$_{55}$ cluster and Ti substituted (four different locations) Mg$_{55}$ cluster.

Table 7.6 Interaction energies of hydrogen with Mg$_{55}$ and TiMg$_{54}$ clusters. The numbers in the parenthesis corresponds to the same for periodic surface.

Table 8.1 Doping of charged alkali and alkaline metal atoms at different positions. In this table 1, 2, 3, 4 locations are Convex surface of central five member ring, Concave surface of central five member ring, Convex surface of side six member ring and Concave surface of side six member ring, respectively.

Table 8.2 Charge on Si, C and H atom of different SiC conformers.

Table 8.3 The average interaction energy/hydrogen molecule and the charge on the Ti atom, when the hydrogen molecule interacts one by one with Ti@SiC_sh.

Table 8.4 The structural parameters and energetics of Sc$_8$C$_{12}$, Ti$_8$C$_{12}$, V$_8$C$_{12}$ clusters.