List of Tables

Table 3.1: Structural parameters and band gap of α-SiX (X=N, P, As, Sb, Bi) monolayers,
respectively
Table 3.2: Comparison of structural parameters and band gap of pristine HGY monolayer with
earlier studies
Table 3.3: Structural parameters and band gap values for Ni@α-SiX SACs with and without H
adsorption conditions, respectively
Table 3.4: Structural parameters and band gap values for transition metals anchored HGY SACs
with and without H adsorption conditions, respectively54
Table 3.5: Löwdin charge (e) analysis of pristine α-SiX (X=N, P, As, Sb, Bi), Ni@α-SiX SACs
and H adsorbed Ni@α-SiX SACs, respectively
Table 3.6: The Löwdin charge analysis of the pristine, transition metals anchored HGY and H
adsorbed transition metals anchored HGY, respectively60
Table 3.7: The obtained adsorption energy and Gibbs free energy of the SACs for HER activity.
61
Table 3.8 The Comparison of calculated Gibbs free energy of HER activity for presented SACs
with previous reports
Table 4.1: Comparison of the calculated bond lengths and band gap of the 2D o-B ₂ N ₂ with
previous reports
Table 4.2: Calculated Gibbs free energy (at pH = 0 to 7) of pristine, defected and C doped 2D
o-B ₂ N ₂ for HER activity94
Table 5.1: The adsorption energy of the first hydrogen molecule over 2D o-B ₂ N ₂ 104
Table 5.2: Binding energy of Na, K, Be, Mg and Ca metals at possible sites of the 2D o-B ₂ N ₂ ,
respectively
Table 5.3: The adsorption energy of the first hydrogen molecule on various sites of B, N, and
BN defected 2D o-B ₂ N ₂ , respectively.
Table 5.4: Binding energy of Sc, Ti, Y and Zr metals at all possible sites of the 2D o-B ₂ N ₂ ,
respectively
Table 5.5: Adsorption energy of the hydrogen molecules over one and two Ti decorated 2D o-
B ₂ N ₂ , respectively
Table 5.6: The comparison of the average adsorption energy per hydrogen molecule and
gravimetric storage capacity of Ti decorated 2D o-B ₂ N ₂ with various reported work118