

## List of Tables

<b>Table 3.1:</b> Optimized lattice constant, bond length, work function, adsorption energy and Gibbs free energy of hydrogen and oxygen of SnSe <sub>2</sub> and doped-SnSe <sub>2</sub> .	<b>55</b>
<b>Table 4.1:</b> Calculated $\Delta E_{ads}^H$ and $\Delta G^H$ of HER activity over pristine and defected SnSe <sub>2</sub> monolayers.	<b>78</b>
<b>Table 4.2:</b> The comparison of $\Delta G^H$ of all stable 2D-TMDs. (Ref. [86])	<b>83</b>
<b>Table 5.1:</b> Calculated lattice and bond lengths of HfS <sub>2</sub> , HfSe <sub>2</sub> and HfSSe monolayers.	<b>100</b>
<b>Table 5.2:</b> Calculated $\Delta E_{ads}^H$ and $\Delta G^H$ of HER activity over pristine HfS <sub>2</sub> , HfSe <sub>2</sub> and HfSSe monolayers.	<b>102</b>
<b>Table 5.3:</b> Calculated lattice, bond lengths, $\Delta E_{ads}^H$ and $\Delta G^H$ of defected HfS <sub>2</sub> , HfSe <sub>2</sub> and HfSSe monolayers.	<b>102</b>
<b>Table 5.4:</b> The comparison of $\Delta G^H$ of all stable 2D-TMDs (Ref. [86]) with HfS <sub>2</sub> and HfSe <sub>2</sub> monolayers (Our Work).	<b>106</b>