

Li adsorption, hydrogen storage and dissociation using monolayer MoS₂: An ab-initio random structure searching approach

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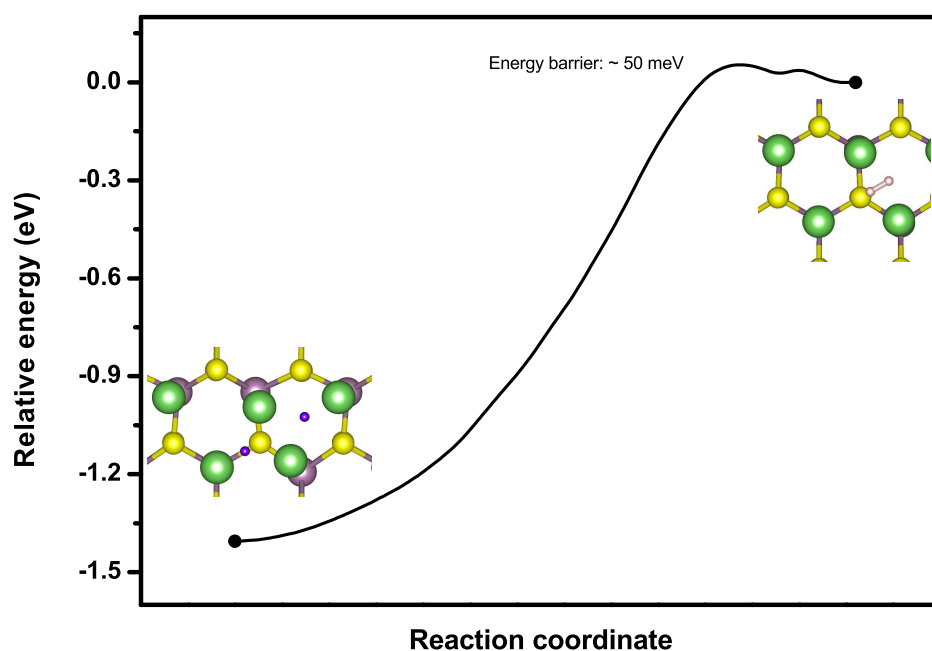


FIG. S1: Path (A) as was shown in Figure 8 detailing the onset of hydrogen molecule dissociation into two triply-coordinated H atoms with Li. An energy barrier of approximately 50 meV was obtained.