Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Quasiclassical Trajectory Calculations of Hydrogen Absorption in the $(NaAlH_4)_2Ti$ System on a Model Analytical Potential Energy Surface

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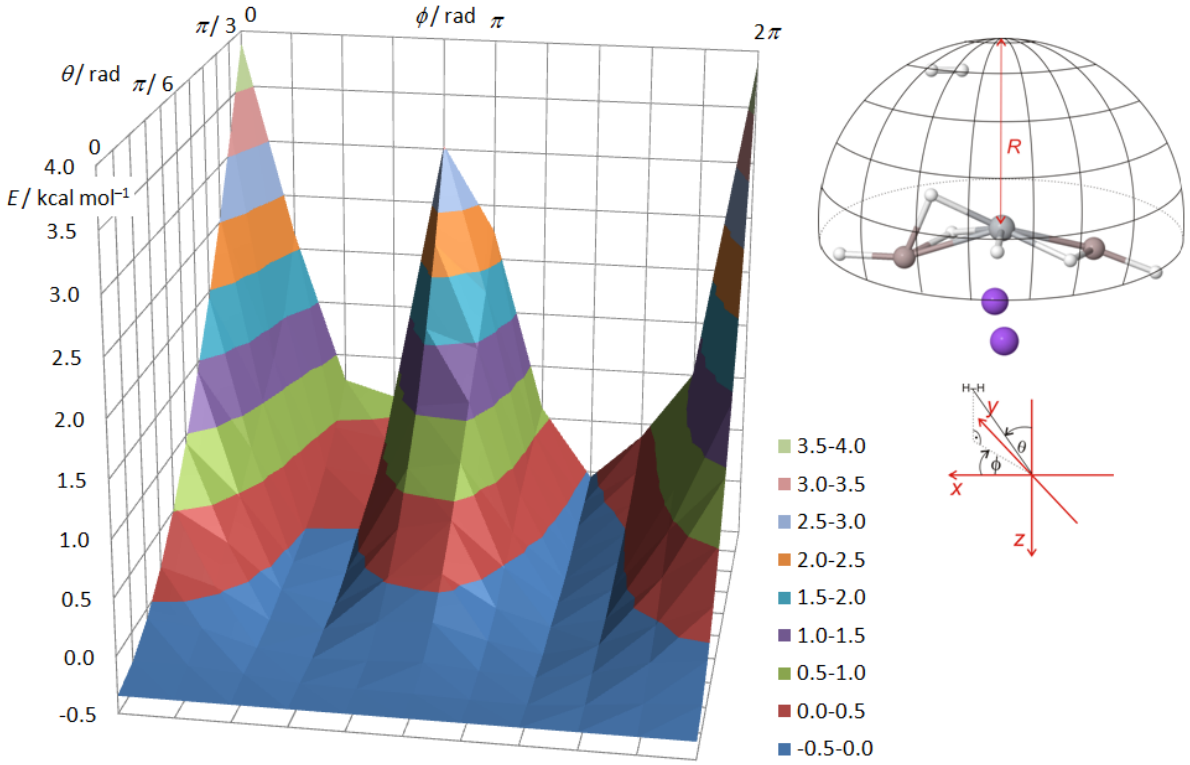

Figure S1. 3D surface plot of the B97-2/6-311++G(2d,p) potential corresponding to the H_2 centre of mass located on the radial grid (R = 4 Å). The H_2 molecule is kept parallel to the x-axis ($d(H_2)$ = 0.74 Å). The zero reference energy corresponds to the H_2 far away from the cluster in the equilibrium geometry.

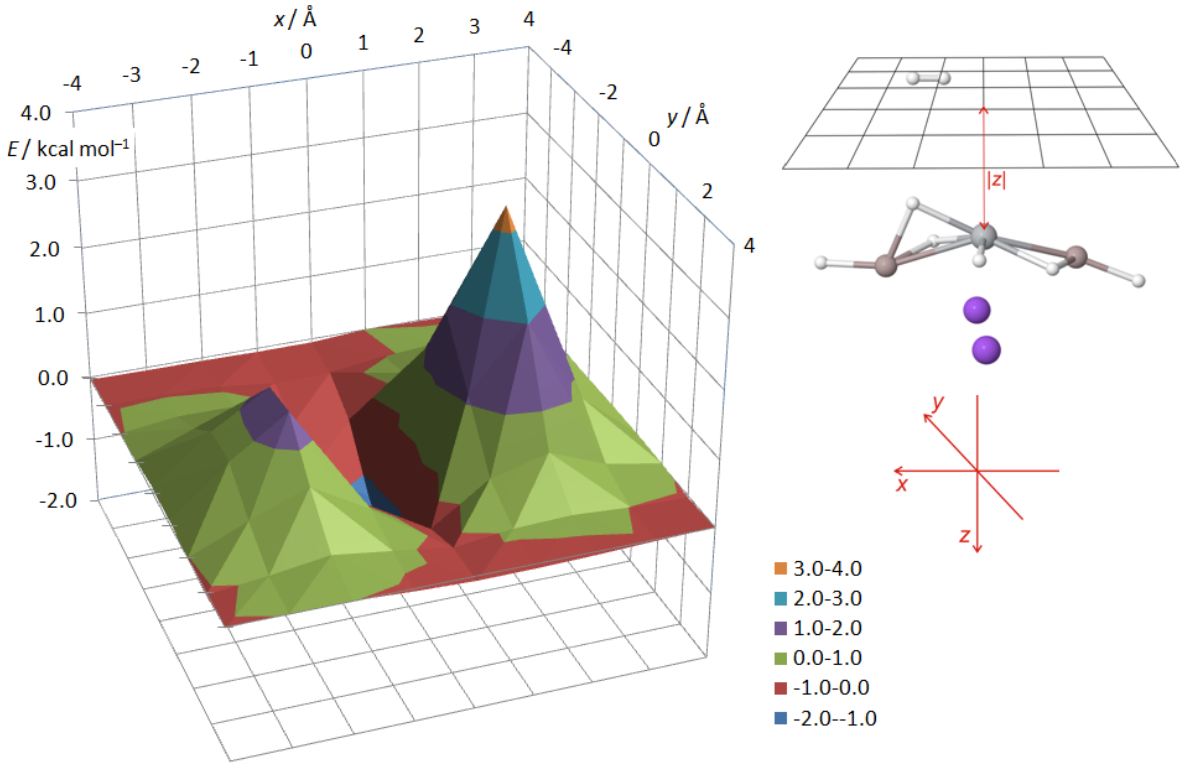

Figure S2. 3D surface plot of the B97-2/6-311++G(2d,p) potential corresponding to the H_2 centre of mass located on the planar grid ($|z|$= 3 Å). The H_2 molecule is kept parallel to the *x*-axis ($d(H_2)$ = 0.74 Å). The zero reference energy corresponds to the H_2 far away from the cluster in the equilibrium geometry.