**Density Functional Theory Study on the Catalytic Dehydrogenation of Methane on MoO3 (010) Surface**

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**Supplementary Information Section**

Table S1: Benchmark calculations for bond dissociation energies of some simple molecules, obtained at PBE-D/TZP level of theory. Dashes in molecules represent the broken bond. ZPE = zero-point energy. Experimental values were obtained from (Y.-R. Luo, Comprehensive handbook of chemical bond energies, CRC press, Boca Raton, Florida, USA, 2007).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Molecule** | **Exp. BDE** | **Calculated BDE (no ZPE)** | **Calculated BDE (ZPE included)** | **% Error (no ZPE)** | **% Error (ZPE included)** |
| H-OH | 497.1 | 515.8 | 483.0 | 3.8% | 2.8% |
| NH2-H | 450.1 | 472.4 | 433.5 | 4.9% | 3.7% |
| H-H | 435.8 | 435.7 | 435.7 | 0.0% | 0.0% |
| CH3-H | 439.3 | 459.9 | 423.1 | 4.7% | 3.7% |
| CH3CH2–H | 420.5 | 439.8 | 402.5 | 4.6% | 4.3% |
| CH3-CH3 | 377.4 | 409.0 | 373.1 | 8.4% | 1.1% |
|  |  |  |  |  |  |
|  |  |  | **Ave. Error** | **4.4%** | **2.6%** |

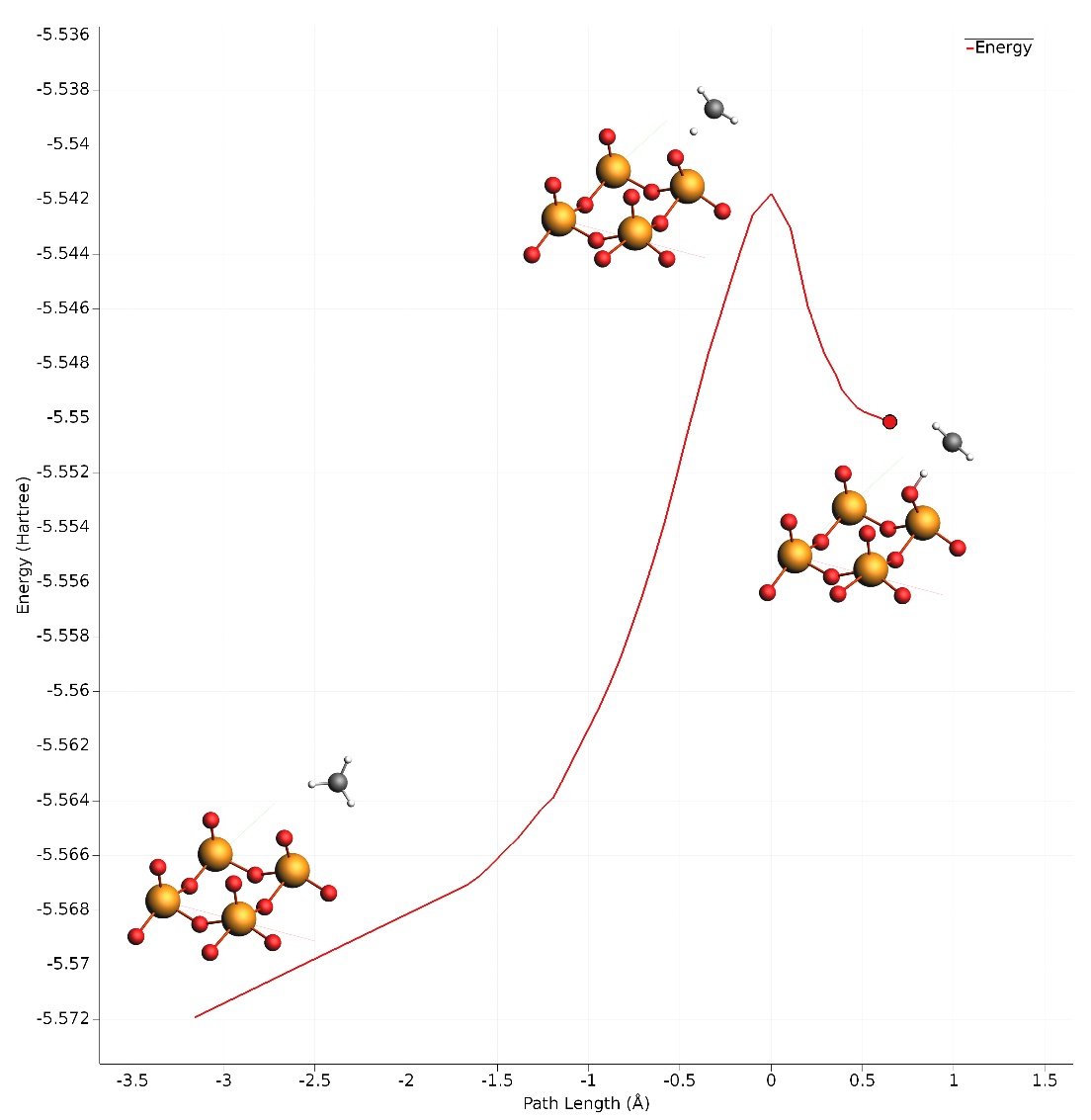


Fig. S1. Intrinsic reaction coordinate (IRC) for the transition state TS1, obtained at PBE-D/TZP level of theory.