I. SUPPLEMENTARY MATERIAL



FIG. 1. The onset potential for the protonation of a nitrogen adatom on the $Mo_{13}N_{13}$ nanocluster structure. For the bridge site, the light dashed line, the onset potential is -1 V and for the three-fold site, the dark filled line, the onset potential is -0.8 V.



FIG. 2. The onset potential for the protonation of a nitrogen adatom on the $Mo_{13}N_{10}$ nanocluster structure. For the bridge site, the light filled line, the onset potential is -0.8 V and for the three-fold site, the dark filled line, the onset potential is -0.65 V.



FIG. 3. The onset potential for the protonation of two nitrogen adatom on the Mo_{13} nanocluster structure.



FIG. 4. The activation barrier for splitting N_2 on the clean molybdenum particle determined using NEB calculations. The barrier is 1.8 eV and dissociation of N_2 on the clean molybdenum will not happen at room temperatures.