Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

On the possibility of an Eley-Rideal mechanism for ammonia synthesis on Mn_6N_{5+x} (x=1)-(111) surfaces

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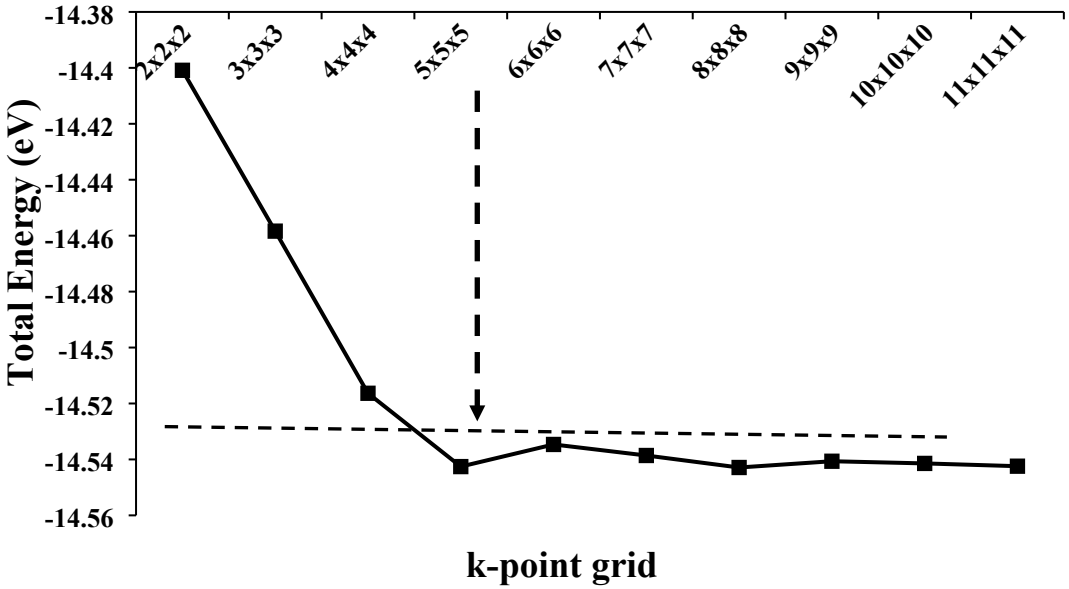
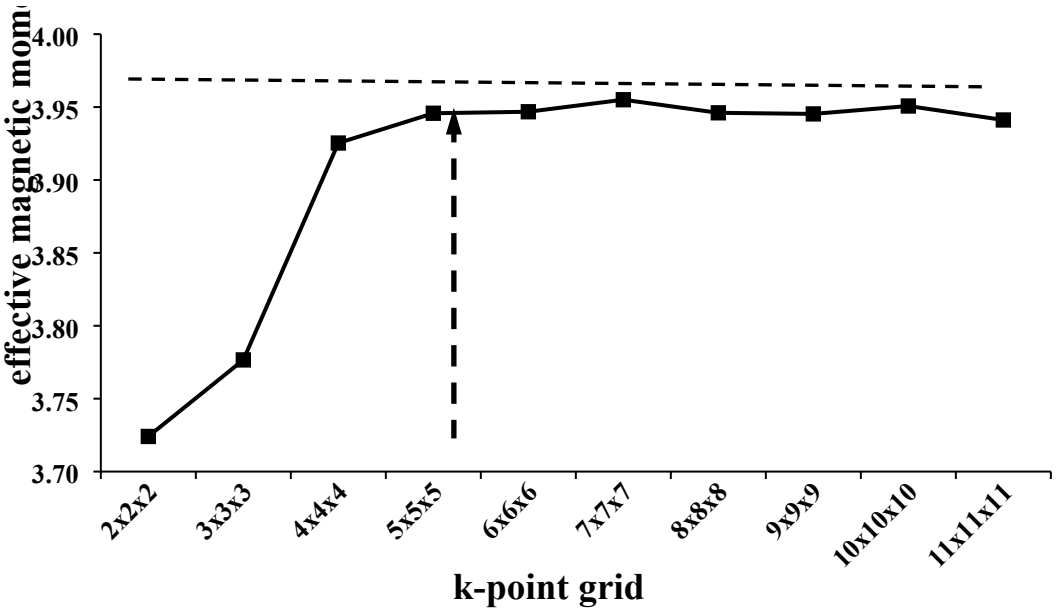


S-Fig. 1 Bulk θ-Mn_6N_5 convergence of energy as a function of k-point grid density.



S-Fig. 2 Bulk θ-Mn_6N_5 convergence of effective magnetic moment as a function of MP k-point grid density.

Based on the convergence observed of the k-point grid and the effective magentic moment per manganese atom observed for the bulk θ-Mn_6N_5 we have calculated the k-point grid for the various slabs of this material. These are shown in the following table.

S-Table 1. k-point grid used to model the various surface slabs of θ-Mn_6N_5

k-points	Surface
3x3x1	**1 0 0**
2x2x1	**1 1 1**
2x2x1	**(1 1 1)'**
3x2x1	**1 1 0**