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

Supporting Information for "Pyrimidine and s-Triazine as Structural Motifs for Ordered Adsorption on Si(100): a First Principles Study "

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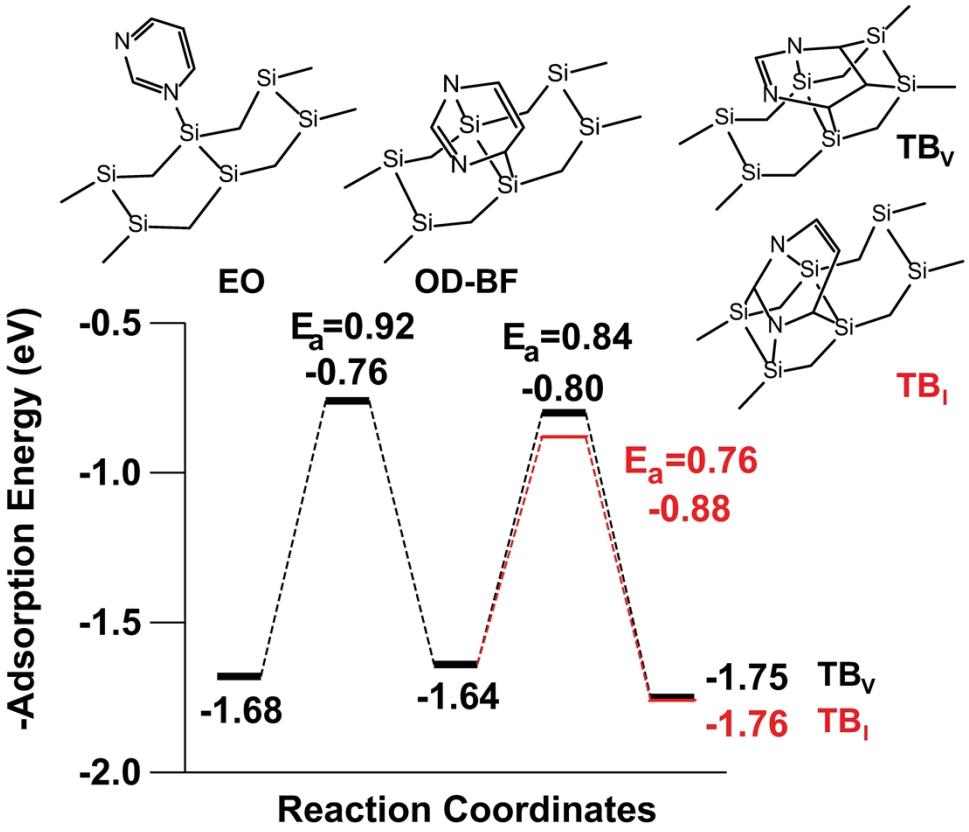

Fig.1 On-dimer [4+2] addition paths of pyrimidine End-On structure followed by tight-bridge formation.

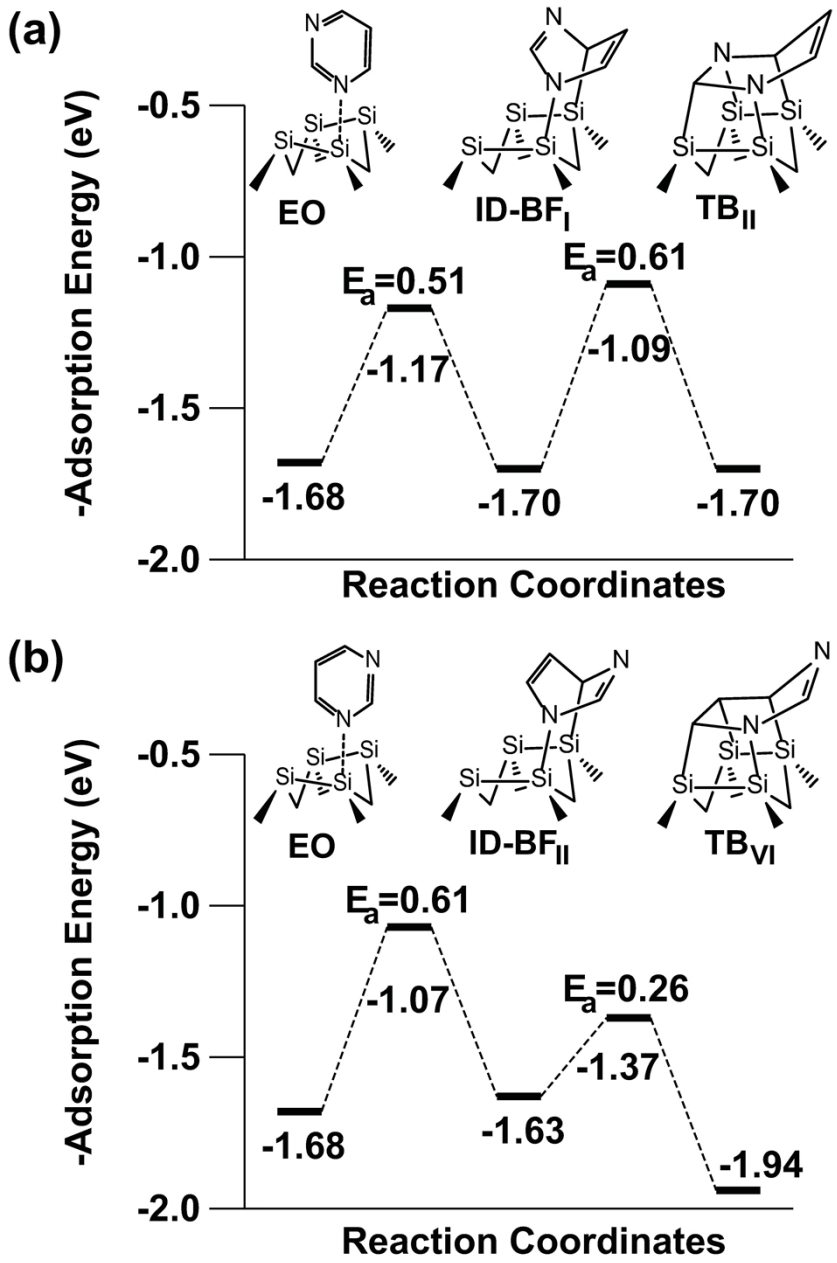

Fig.2 Interdimer [4+2] addition paths of pyrimidine End-On structure followed by tight-bridge formation.

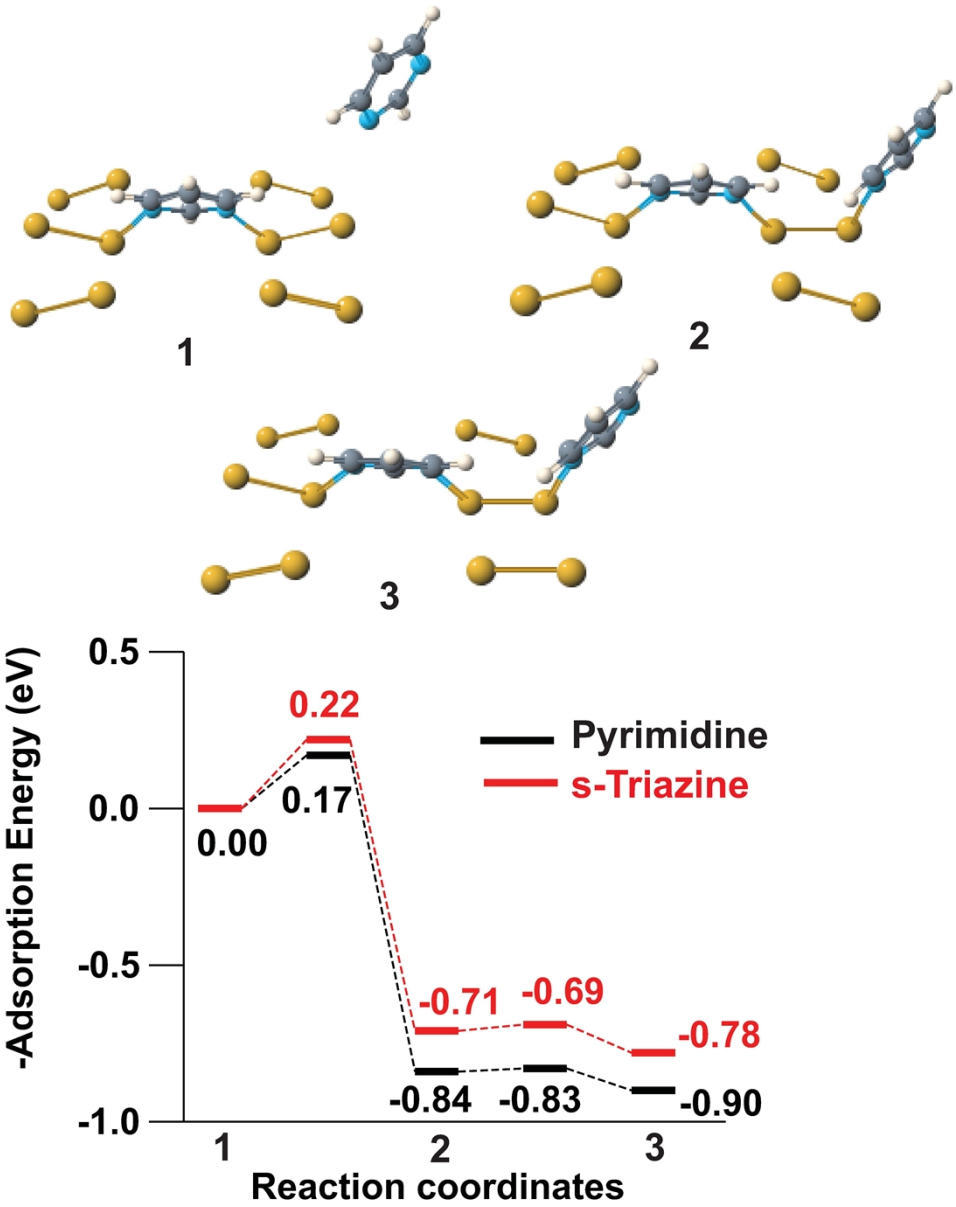

Fig.3 The formation of 1D line by NN-CRB structure. There is a barrier for the formation of the N-Si dative bond, since the Si atom is tilted up. These reactions are simulated using a 4x4 unit cell. Only 6 of the dimers and the two molecules are shown.

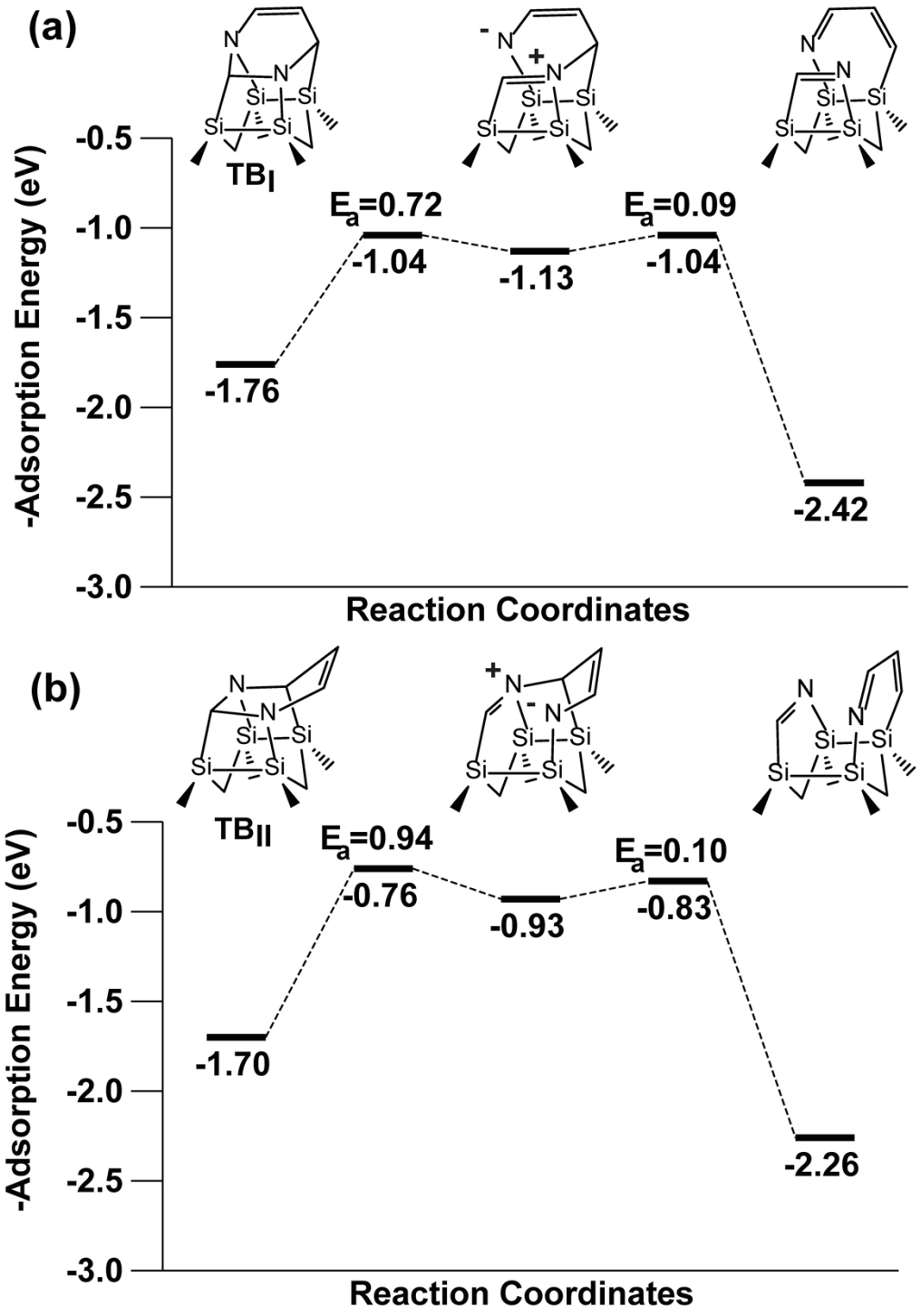

Fig.4 Two decomposition paths of pyrimidine on surface with the lowest barriers.

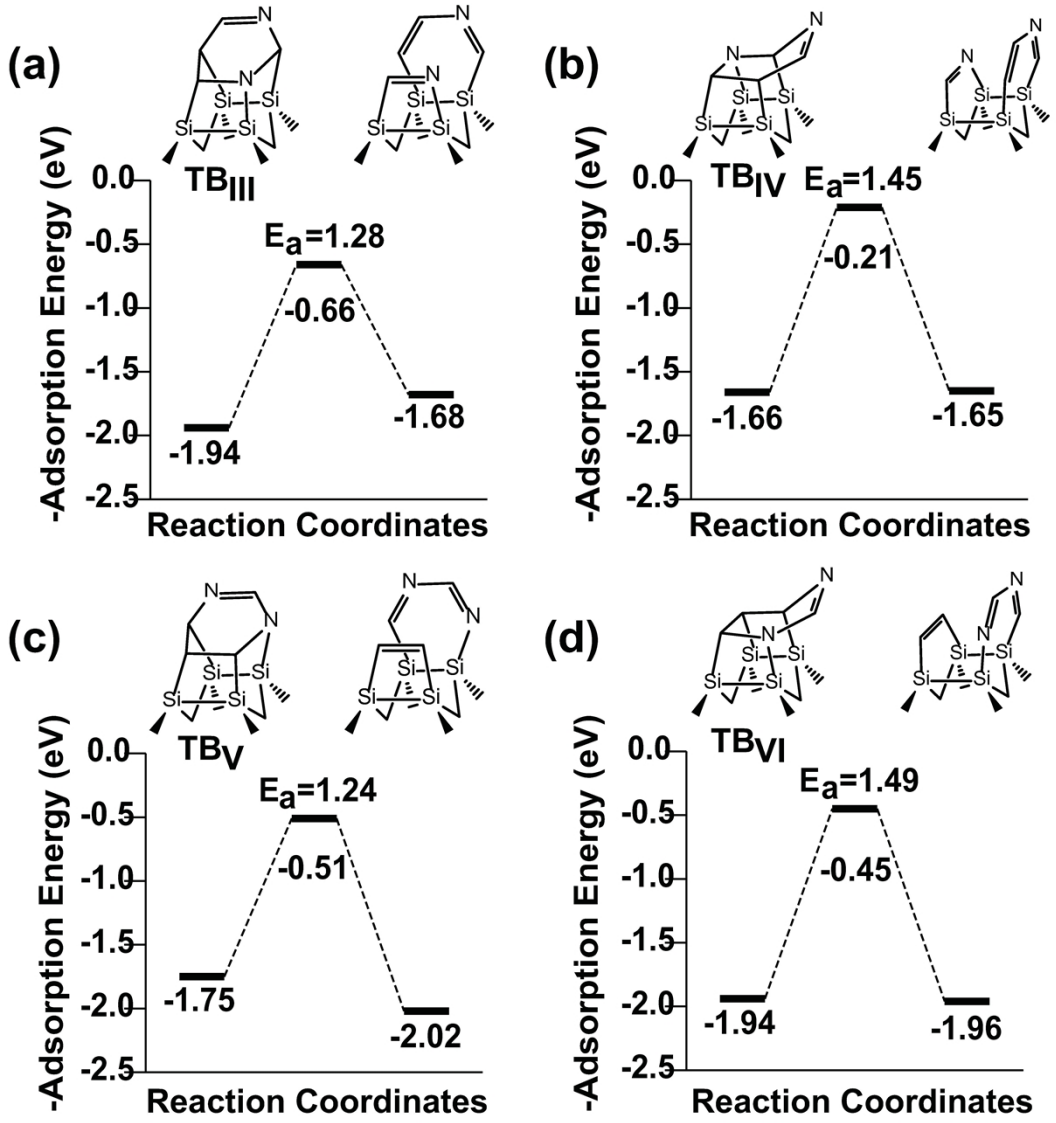

Fig.5 Four other decomposition paths of pyrimidine on surface with higher barrier.

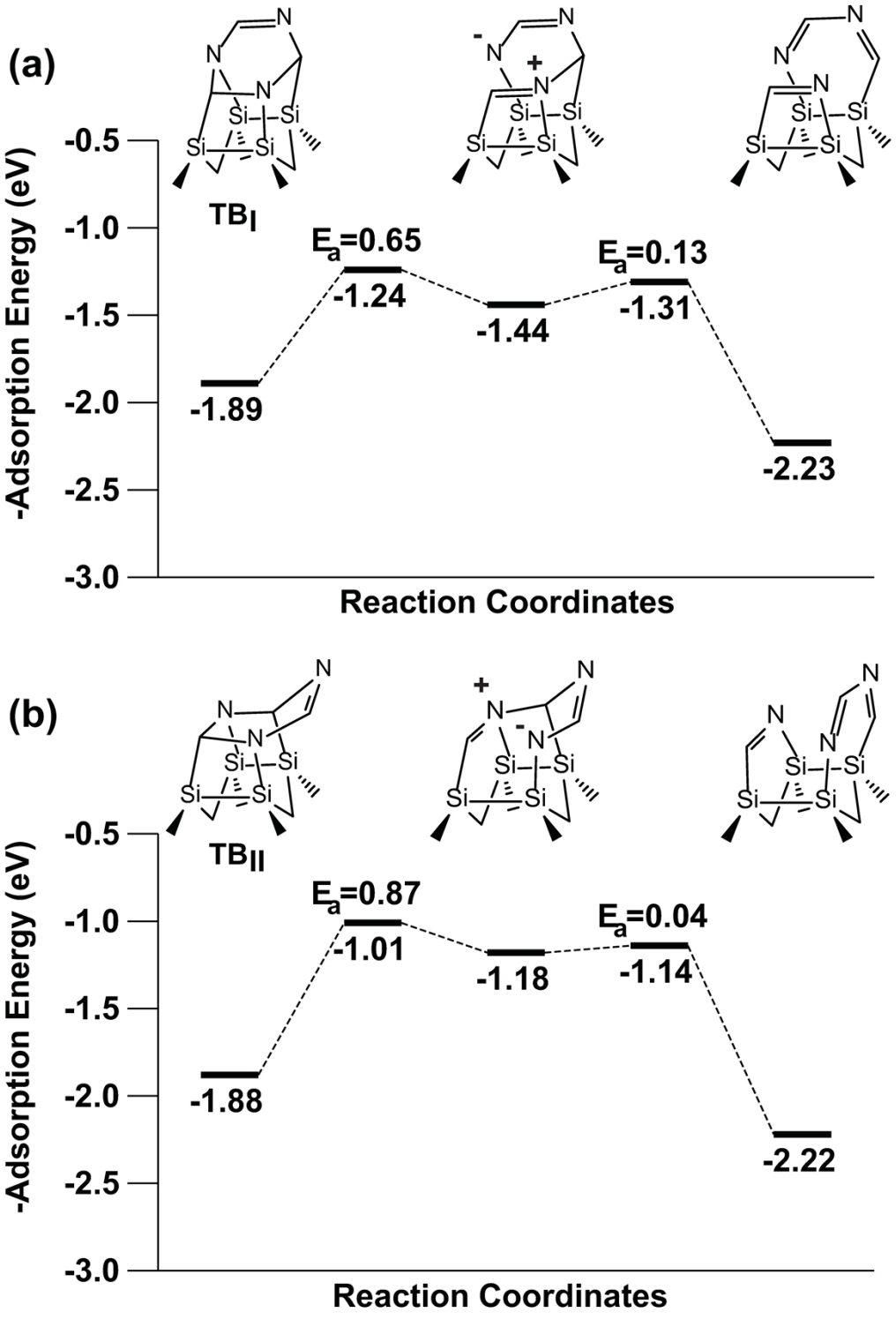

Fig.6 Decomposition paths for s-triazine adsorbed on Si(100).