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

Wilson K.H. Ng¹, J.W. Liu², and Zhi-Feng Liu¹,*

¹Department of Chemistry

and

Centre for Scientific Modeling and Computation

Chinese University of Hong Kong

Shatin, Hong Kong, China

and

²National Supercomputing Center in Shenzhen

Shenzhen, China

*To who correspondence should be addressed. Email: zfliu@cuhk.edu.hk fax: ++852-2603-5057
Contents

On-dimer [4+2] addition paths for pyrimidine .......................................................... 3
Interdimer [4+2] addition paths for pyrimidine ....................................................... 4
Path for the formation of a dative bond next to a NN-CRB structure .................... 5
Decomposition paths for pyrimidine ....................................................................... 6, 7
Decomposition paths for s-triazine ......................................................................... 8
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).