Electronic Supplementary Information (ESI) for Nanoscale

Rapid Atomic Layer Deposition of Silica Nanolaminates: Synergistic Catalysis of Lewis/Brønsted Acid Sites and Interfacial Interactions

Guoyong Fang$^{ab}$, Jing Ma$^a$*

Email: majing@nju.edu.cn

$^a$Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry of Ministry of Education, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China

$^b$College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325035, P. R. China

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Figure S1. Potential energy profile for (A) **TMA reaction** on the hydroxylated SiO$_2$ substrate, represented by the slab model, Si$_{48}$O$_{30}$H$_{24}$-(OH)$_{12}$, and the cluster model I, Si$_{49}$O$_{30}$H$_{40}$-(OH)$_{12}$, at the PBE/DNP level. For **substrate**, TS$^{A}$, TS$^{2A}$, and P$^{2A}$, the optimized structures, by using slab and cluster models, respectively, are shown in insets. The cell size is also given.
**Figure S2.** The optimized structures of $\text{TS3}^B$ and $\text{TS2}^C$, where the surface reconstruction and interfacial interactions between reactants and the second layer of surface are displayed.
Figure S3. Potential energy profile for (A) TMA reaction.

Figure S4. Potential energy profile for (B) silanol reaction.
Figure S5. Potential energy profile for (C) propagation reaction.

Figure S6. Gibbs free energy (500K) and potential energy (0K) profiles for (D) cross-linking reaction.