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Supporting Information

A Novel Approach to Controlling $CaCO_3$ Crystalline Assembly by Changing the Concentration of Poly(aspartic acid)

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Models of Calcite surfaces

The space groups of calcite, $CaCO_3$, is R3(-)c and its lattice parameters are a=b=4.9896 Å, c=17.0610 Å, α=β=90 Å and γ=120°.[1] All the force field parameters of the atoms in calcite were assigned under the COMPASS force field. In order to validate the applicability of the COMPASS force field to calcite, we compared the calculated crystals lattice parameters with the literature reported data. The lattice parameters from the force field calculations after the minimization of the calcite are a=b=4.99 Å, c=17.06 Å; α=β=90°, γ=120°, which are very close to the reported in the literature.[1] The comparisons validate the applicability of the COMPASS force field to the calcite crystal structure similation. The calcite crystallographic surfaces were built by cleaving along the (001) and (104) planes, follows by the smart minimizer method under the periodic boundary conditions with a non-bond cutoff distance of 9.5 Å. The smart minimizer method includes the steepest descent method with a convergence of 1000 kcal mol^{-1} $Å^{-1}$, then a conjugate gradient with a convergence of 10 kcal mol^{-1} $Å^{-1}$, and finally the BFGS algorithm with a convergence of 0.1 kcal mol^{-1} $Å^{-1}$. The dimensions of the calcite surface used for the calcite/polymer interface simulations were 43.21 × 24.95 × 8.53 Å for calcite (001), 40.48 × 24.95 × 10.67 Å for calcite (104), as shown in Fig. S1.

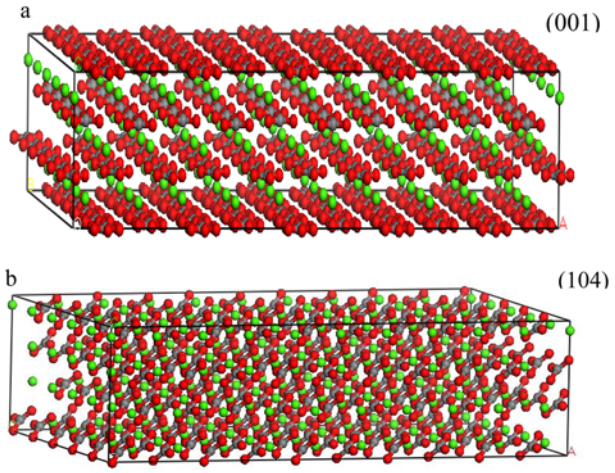

Fig.S1. Ball-and stick models of calcite surface. (a) calcite (001); (b) calcite (104). The dimension unit is Ångström. Color codes: calcium atom, green; carbon atom, gray; and oxygen atom, red.

Models of polymer molecules

Model I. The polymer chains were built with the Amorphous Cell module in the Material studio. For the PVA membrane, the initial atactic polymer chain consisted of 200 repeat units with a 50:50 probability for the occurrence of cis and trans configurations. The packing model with a density of 1.26 g/cm^3 containing one PVA chain was constructed by amorphous cell module.[2] A 5000-step energy minimization was performed at the initial stage to eliminate the bad contact (overlapping or close contact). MD simulations were conducted on this PVA model under the NVT ensemble with a time step of 1fs for 150ps, then additional 150ps MD

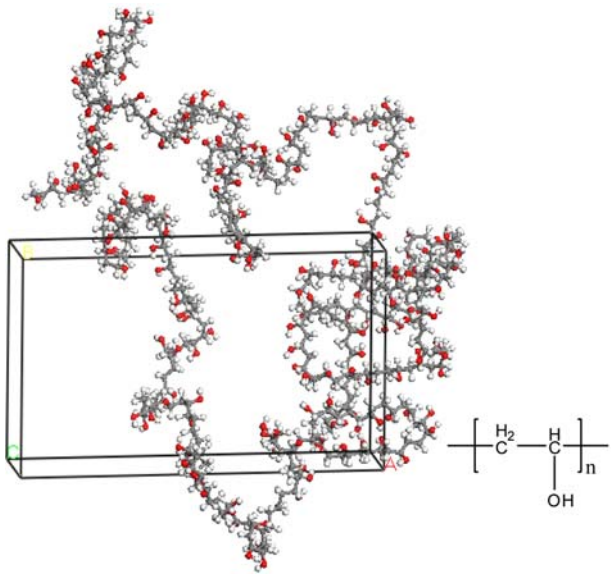

Fig.S2. Tree-dimensional ball-and stick models and the chemical structure of the PVA membrane. Color codes: carbon atom, gray; hydrogen atom, white; and oxygen atom, red.

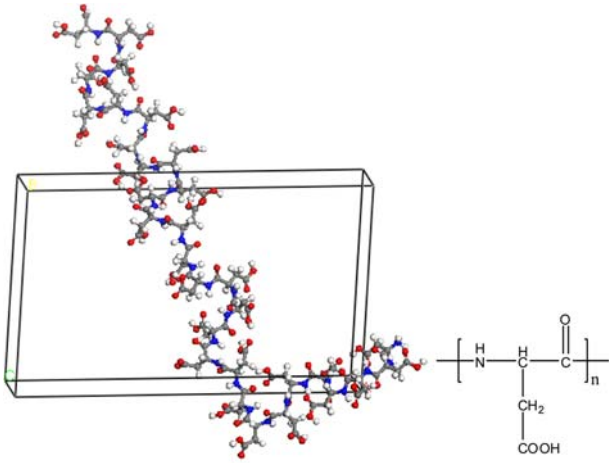

Fig.S3. Tree-dimensional ball-and stick models and the chemical structure of the pAsp molecule. Color codes: carbon atom, gray; hydrogen atom, white; oxygen atom, red; and nitrogen atom, blue.

simulations under the NPT ensemble. This was followed by an annealing procedure by which the systems were heated from 298 K to 373 K at intervals of 15 K and then cooled back. At each step 150ps was applied on the cell. The annealing procedure was performed by the discover module. Afterwards, a 150ps MD equilibration run on the system was performed in the NPT (T=298 K, P=1.01 × 10^5) ensemble to obtain the equilibrium density. Fig. S2 shows the chemical structures and three-dimensional structures of the PVA chain obtained from the MD simulations.

Model II. For the pAsp molecule, the initial homopolymer chain consisted of 30 repeat units with the orientation of Head-to-Tail. The cell containing one pAsp chain was constructed by amorphous cell module. A 5000-step energy minimization was performed at the initial stage to liminate the bad contact (overlapping or close contact). MD calculations was using on this pAsp model in order to obtain the stable configuration, which was conducted for 150ps at 298 K under the canonical ensemble (NTV). Fig.S3 shows the chemical structures and three-dimensional structures of the pAsp chain obtained from the MD simulations.

References

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2. Pan, F.; Peng, F.; Jiang, Z. *Chemical Engineering Science* **2007**, *62*, 703-10.