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Supporting Information
for

Nucleation of Biomimetic Hydroxyapatite Nanoparticles on the Surface of Type I Collagen by Hybrid All-Atom and Coarse-Grained Model

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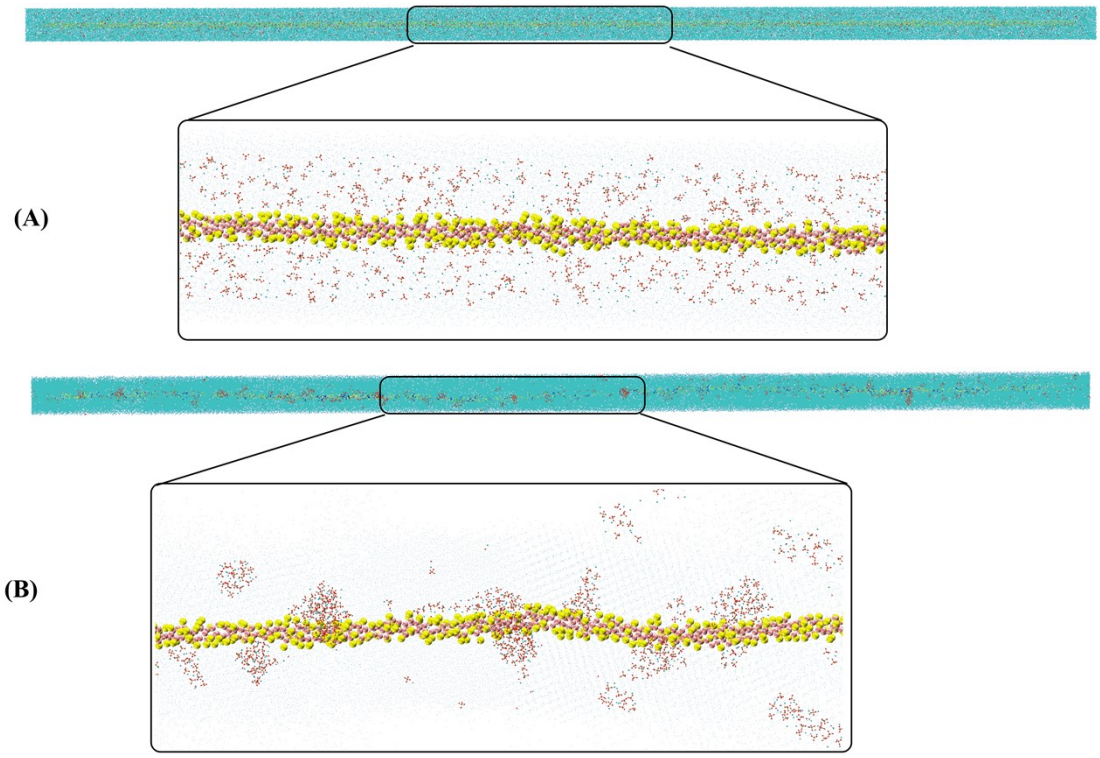
Contents

Figure S1 (A)The details of initial AA/CG model;(B) The details of AA/CG model after 4.5 μs nucleation dynamics. S1
Figure S2 Process diagram of the genetic algorithm (GA). S2
Table S1 Binding energies for each system obtained through metadynamics simulations S3
Table S2 Charges of the residues and the parameter types in the MARTINI force field. S4



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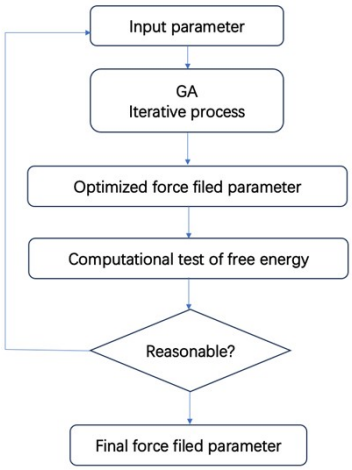

Figure S2 Process diagram of the genetic algorithm (GA).

Table S1 Binding energies for each system obtained through metadynamics simulations

Model	AA	AA/CG
Ca^{2+}/PO_4^{3-}	−7.5	−8.3
CMP-R/PO_4^{3-}	−15.2	−16.5
CMP-K/PO_4^{3-}	−11. 8	−13. 2
CMP-E/Ca^{2+}	−9.2	−10.7
CMP-D/Ca^{2+}	−8.1	−9.9

Units are in kcal/mol

Table S2 Charges of the residues and the parameter types in the MARTINI force field.

Residue	Types	Charge
Arg	SQ3p	1.0
Lys	SQ4p	1.0
Glu	Q5n	−1.0
Asp	SQ5n	−1.0