Supporting Information for

Thermal Annealing of SiC Nanoparticles Induces SWNT Nucleation: Evidence for a Catalyst-Independent VSS Mechanism

Alister J. Page[1], K. R. S. Chandrakumar[1], Stephan Irle*[,2] and Keiji Morokuma*[,1,3]

[1]*Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan*

[2]*Institute for Advanced Research and Department of Chemistry, Nagoya University, Nagoya 464-8602, Japan*

[3]*Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, Atlanta, GA 30322, U.S.A.*

*To whom all correspondence should be addressed. E-mail: sirle@iar.nagoya-u.ac.jp (S. I.); morokuma@fukui.kyoto-u.ac.jp (K. M.)

Movie S1. SWNT cap formation observed in trajectory $8_{2500K\text{-}small1}$, between 90 and 150 ps. Blue and cyan spheres represent Si and C atoms, respectively. Yellow spheres represent carbon atoms eventually involved in polygonal carbon ring formation.

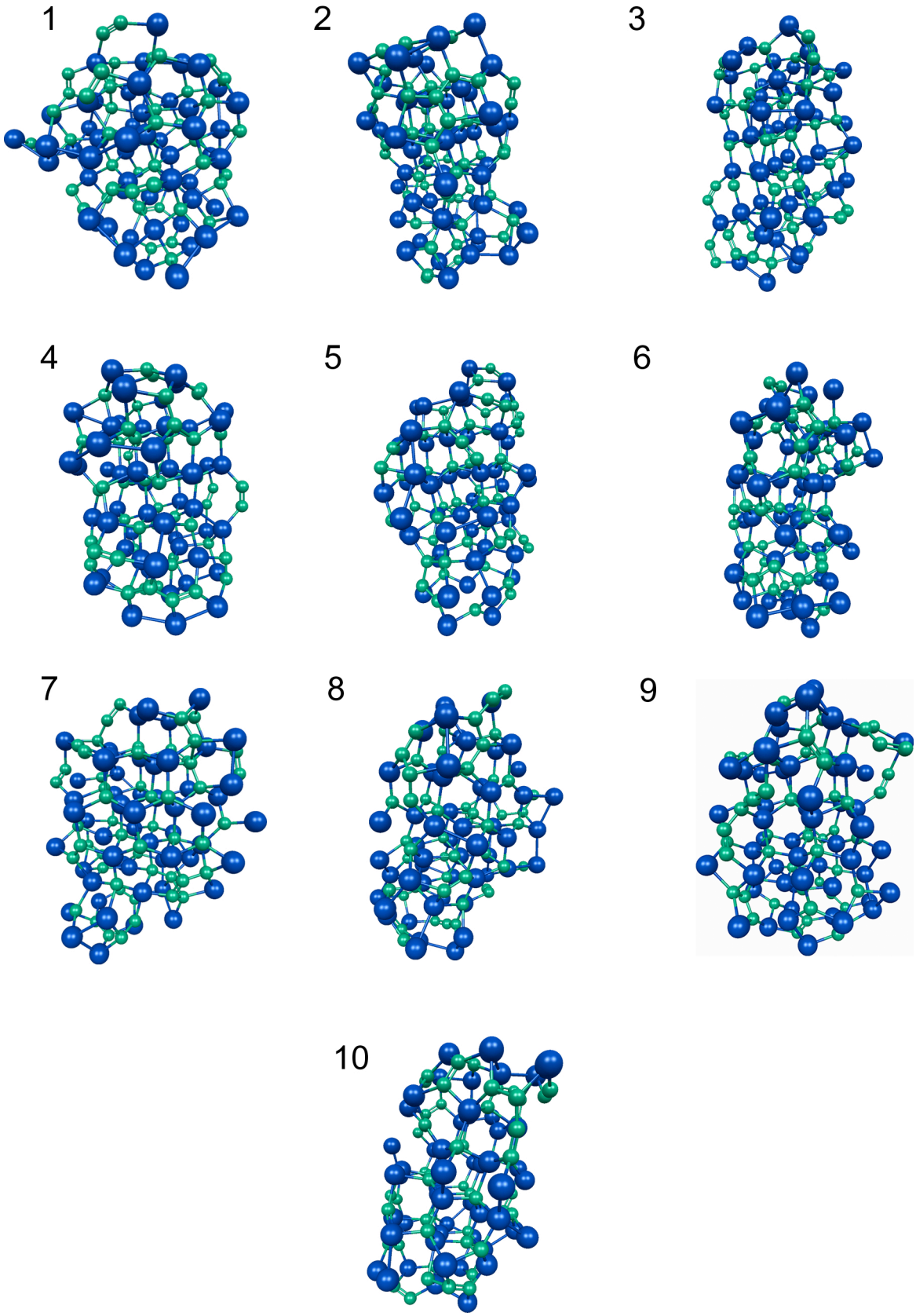

Figure S1. Structures of trajectories $1_{1200K\text{-}small}$-$10_{1200K\text{-}small}$ after 250 ps of SCC-DFTB/MD simulation. Blue and cyan spheres represent Si and C atoms, respectively.

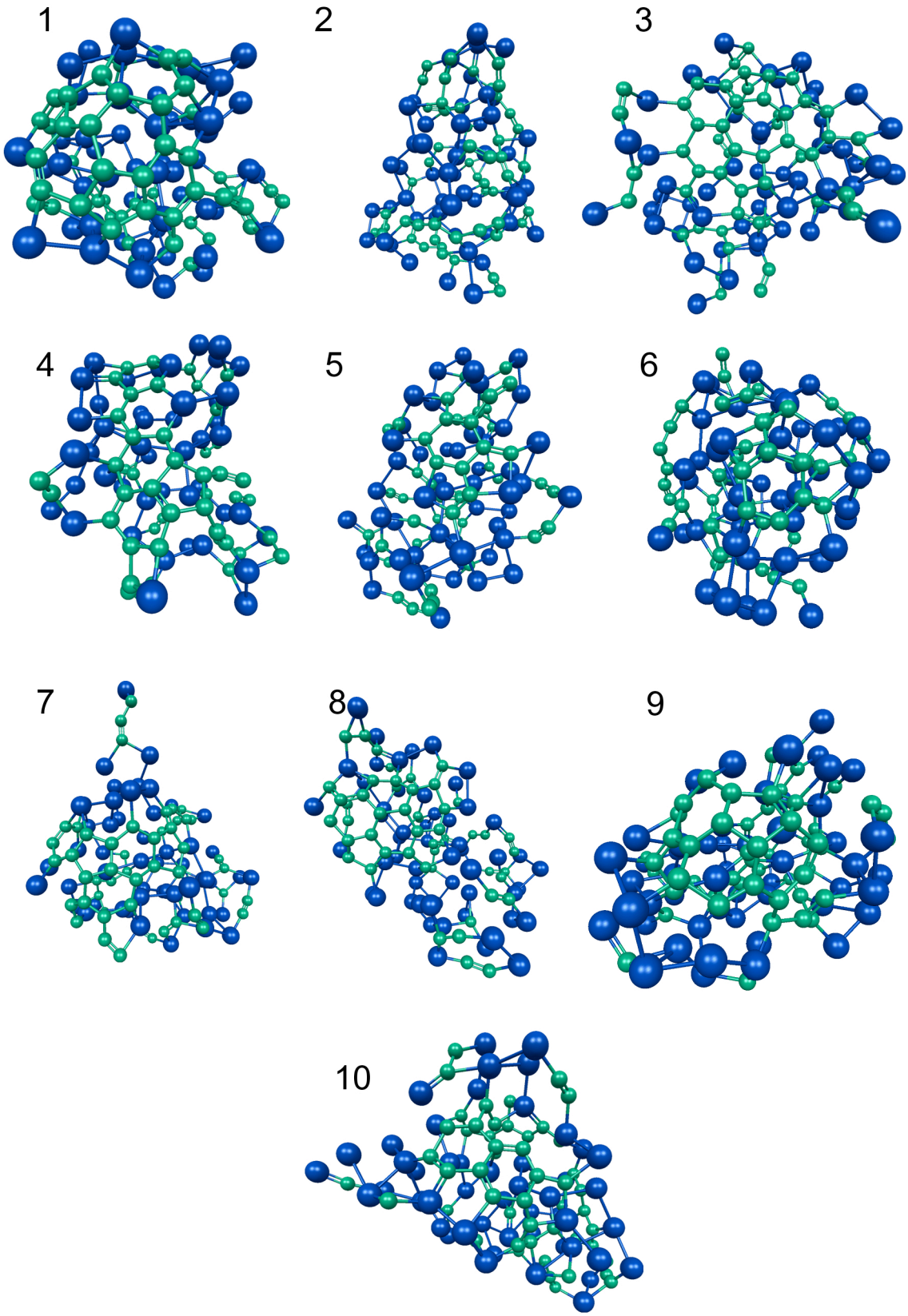

Figure S2. Structures of trajectories $1_{2500K\text{-}small}$-$10_{2500K\text{-}small}$ after 250 ps of SCC-DFTB/MD simulation. Color conventions as in Figure S1.

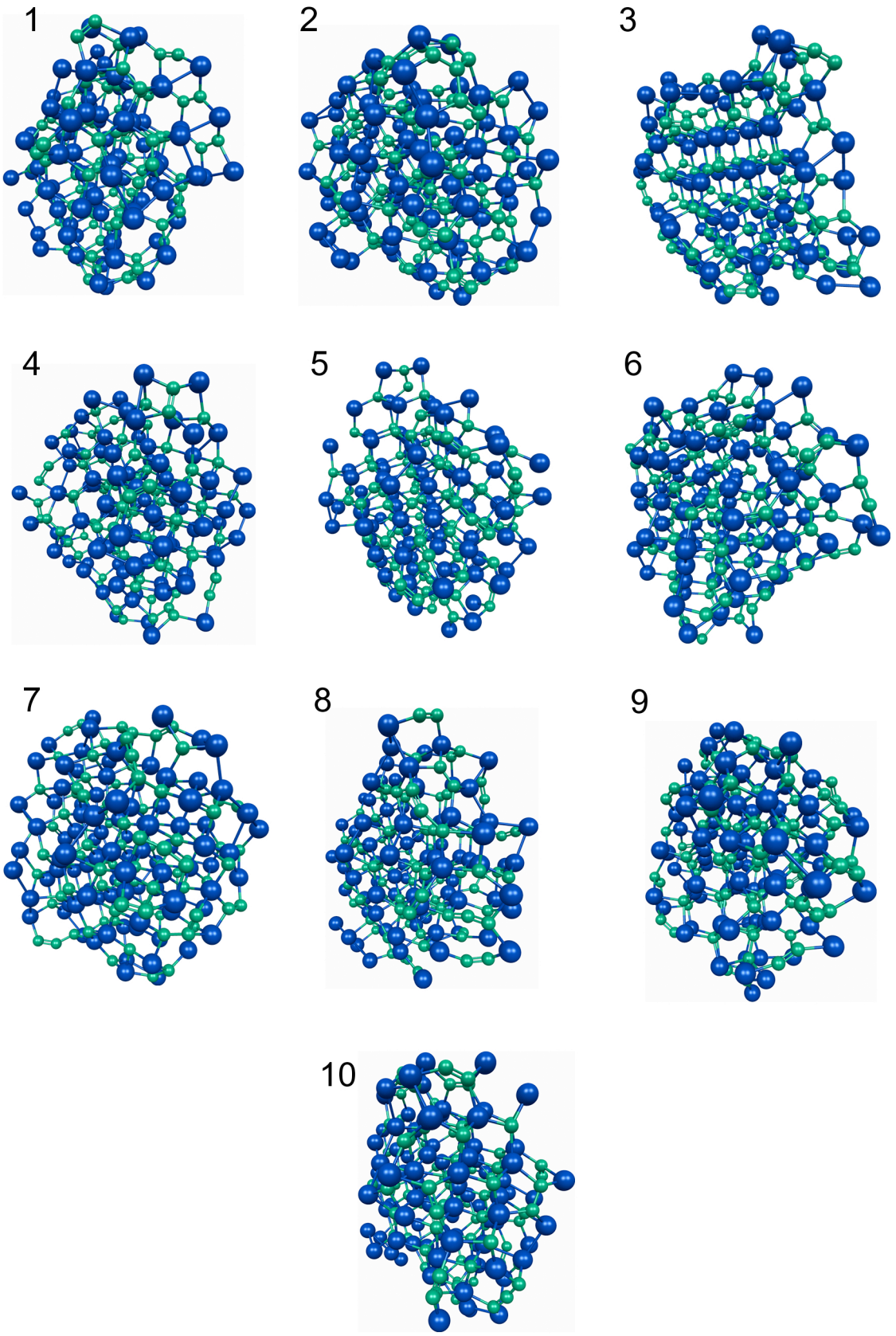

Figure S3. Structures of trajectories $1_{1200K\text{-}large}$-$10_{1200K\text{-}large}$ after 250 ps of SCC-DFTB/MD simulation. Color conventions as in Figure S1.

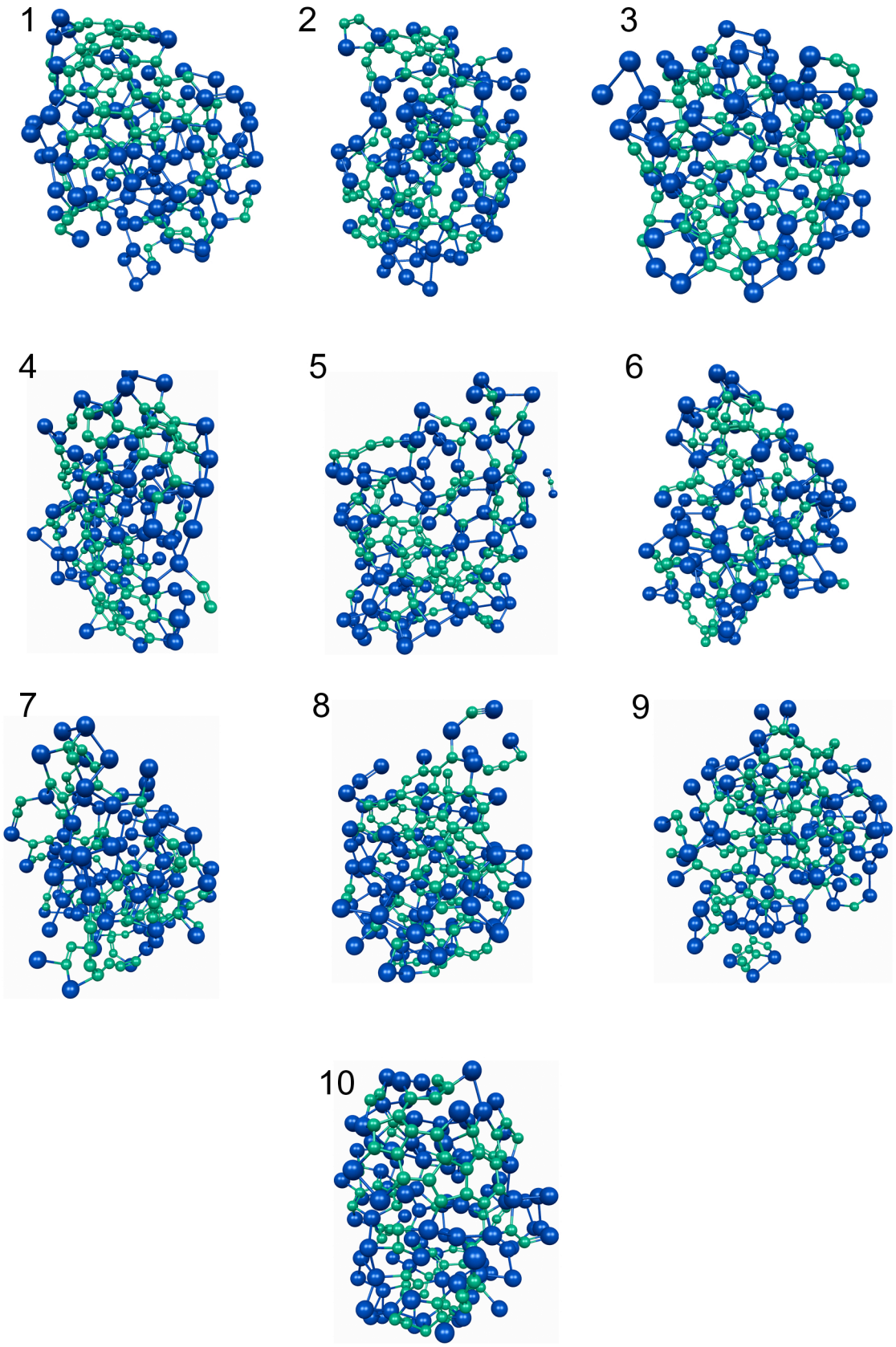

Figure S4. Structures of trajectories $1_{2500K\text{-}large}$-$10_{2500K\text{-}large}$ after 250 ps of SCC-DFTB/MD simulation. Color conventions as in Figure S1.

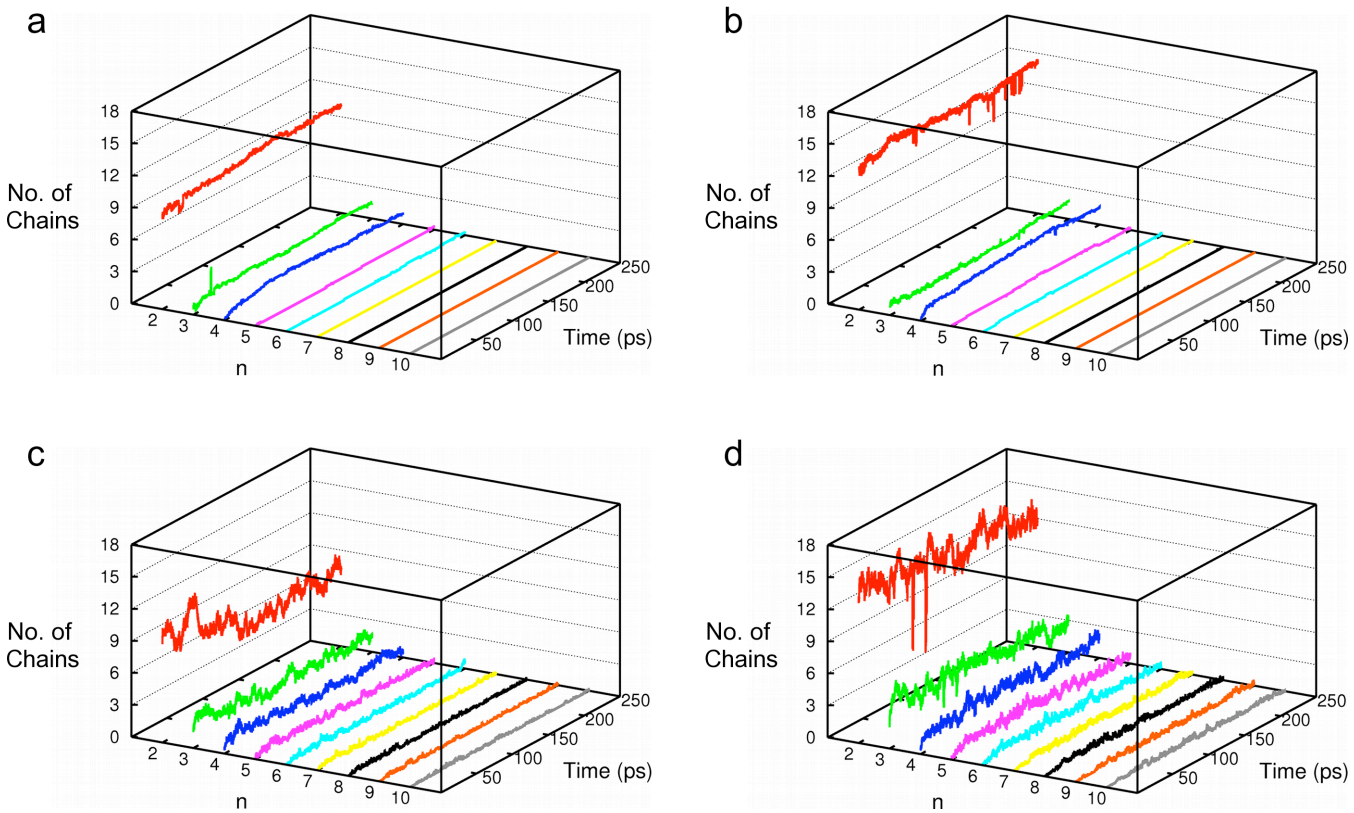

Figure S5. Average C_n chain populations for a) small SiC at 1200 K, b) large SiC at 1200 K, c) small SiC at 2500 K and d) large SiC at 2500 K.

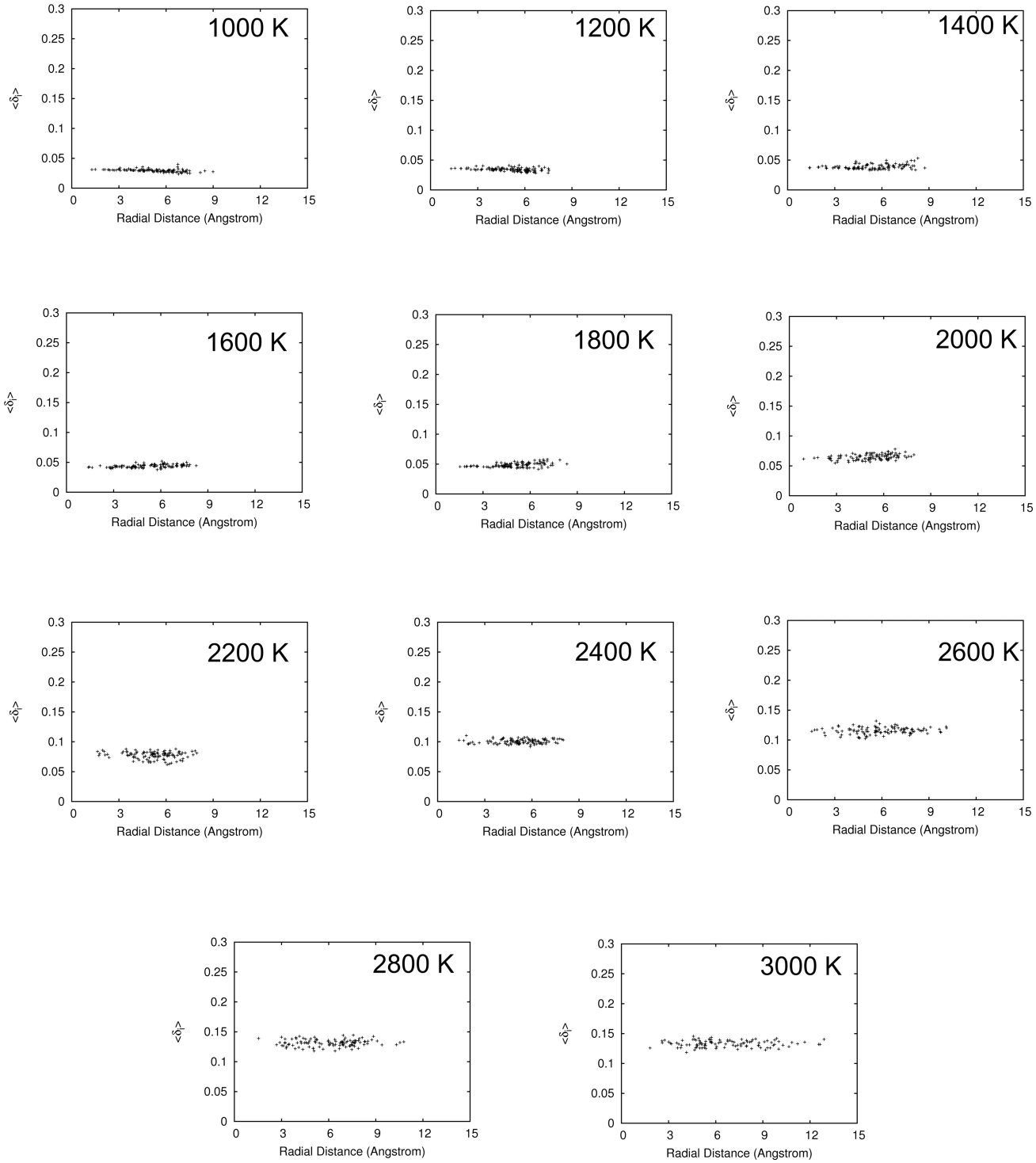

Figure S6. $\langle\delta_i\rangle$ for small SiC nanoparticles between 1000 – 3000 K.

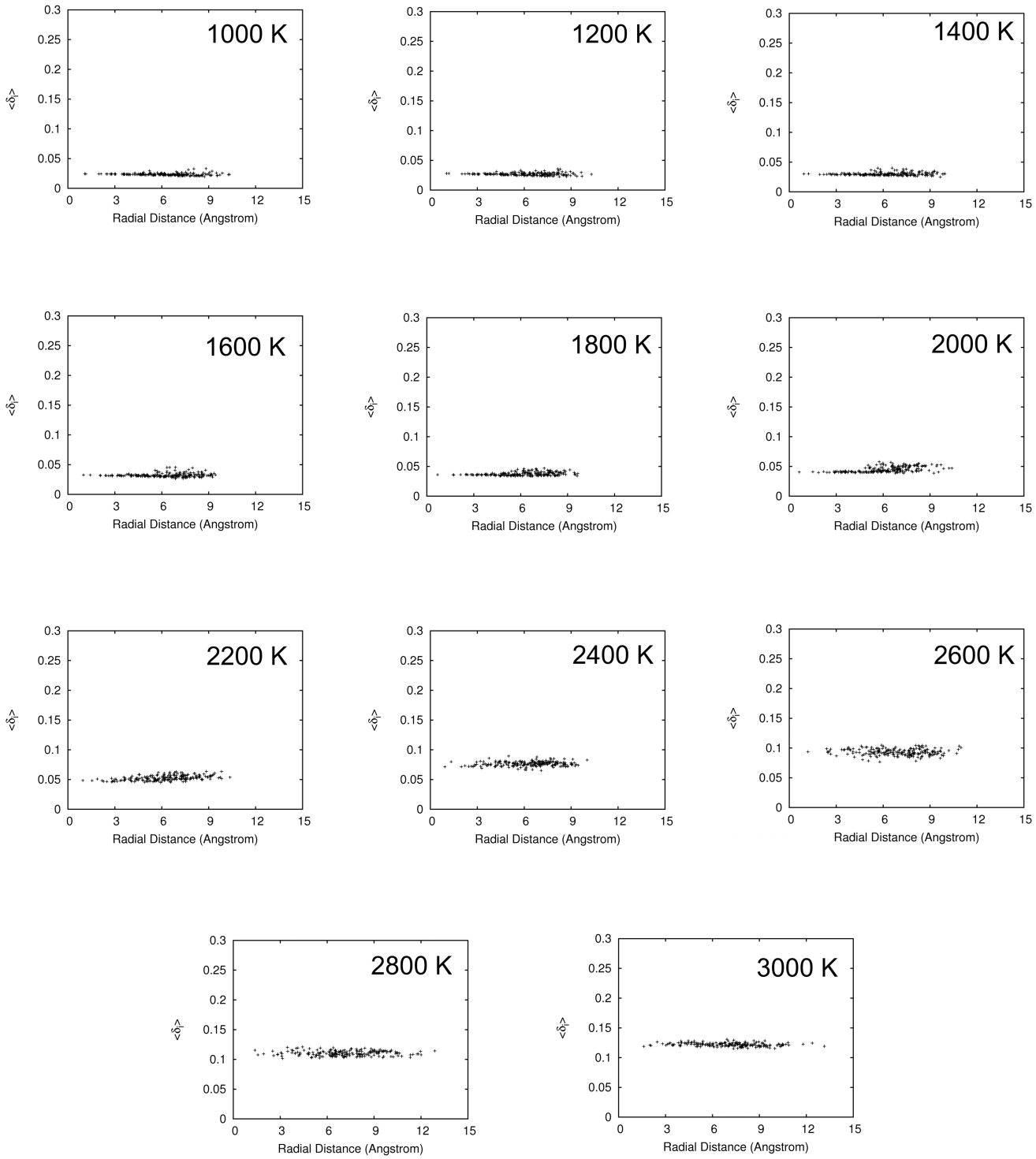

Figure S7. $\langle\delta_i\rangle$ for large SiC nanoparticles between 1000 – 3000 K.