Supporting Information for:

High-Temperature Transformation of Fe-Decorated Single-Wall Carbon Nanohorns to Nanooysters: A Combined Experimental and Theoretical Study

K. R. S. Chandrakumar,[a] Jason D. Readle,[c] Chris Rouleau,[c] Alex Puretzky,[c] David B. Geohegan,*[c] Karren More[c], Veena Krishnan,[d] Mengkun Tian,[d] Gerd Duscher,[c,d] Bobby Sumpter,[c] Stephan Irle,*[b] and Keiji Morokuma*[a]

[a]*Fukui Institute of Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan*
[b]*Institute for Advanced Research and Department of Chemistry, Nagoya University, Nagoya 464-8602, Japan*
[c]*Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A.*
[d]*University of Tennessee, Knoxville, TN, U.S.A.*

Table of Contents

· Corresponding Authors. E-Mail addresses: geohegandb@ornl.gov (D.B.G.), sirle@chem.nagoya-u.ac.jp (S.I.), keiji.morokuma@emory.edu (K.M.)

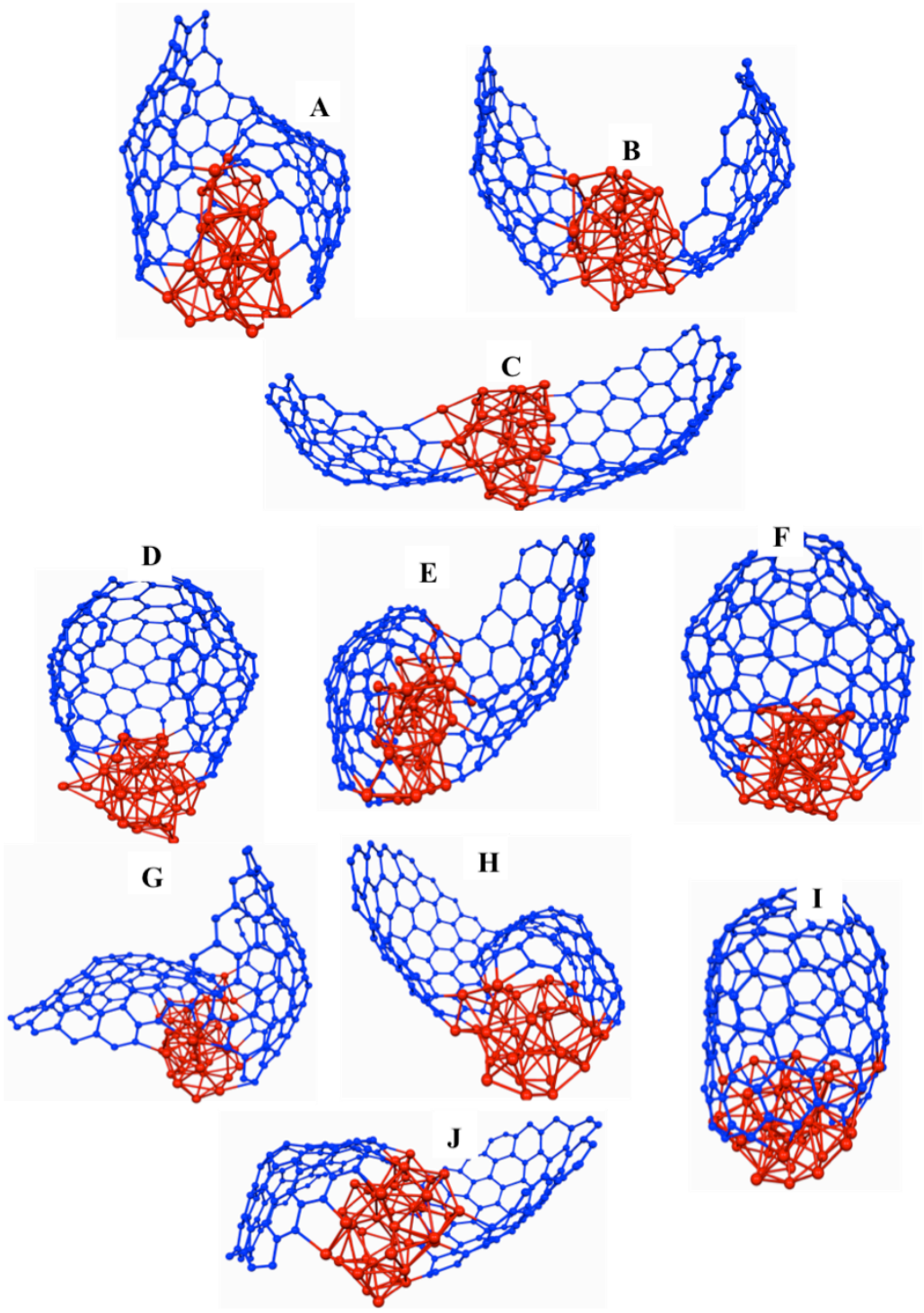

Figure S1. The structures obtained at 1500 K at the trajectory endpoints. Different trajectories are identified by Roman letters A-J, and the trajectory runtime is up to at least 32 ps.

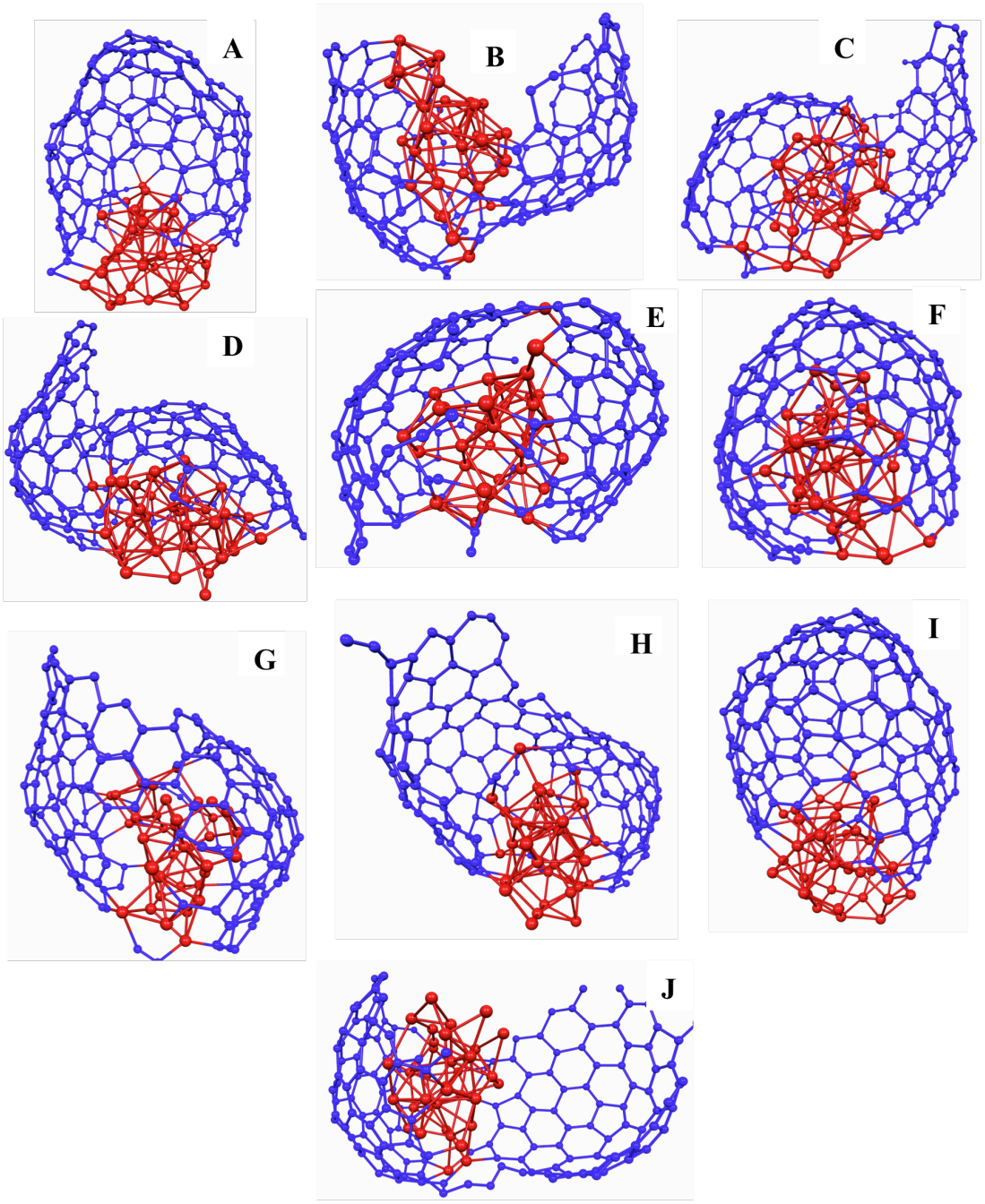

Figure S2. The structures obtained at 2500 K at the trajectory endpoints. Different trajectories are identified by Roman letters A-J, and the trajectory runtime is up to at least 43 ps.