Electronic Supplementary Information

The Largest Fullerene

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Effects of defects in fullerenes

The effects that defects have on the potential energy of single-caged fullerenes were investigated by preparing structures with three separate types of defects: 1) *Bond rotation*, where a pair of C neighboring atoms are rotated by 90 degrees around the center of their connecting. This leads to four adjacent hexagons being converted into two pentagons and two heptagons. 2) *Single vacancy*, where a single C atom is removed from the carbon lattice. 3) *Double vacancy*, where two adjacent C atoms are removed. All three of these cases were tested at the center of the 20 facets of an icosahedral fullerene as a function of the molecular sizes (number of atoms, N). Following the introduction of the defects, the structures were optimized using the same methods as for the intact fullerenes. The resulting excess energy caused by these defects are shown in Figure A for fullerenes ranging in size from 240 to 6,000 atoms in their pristine form.

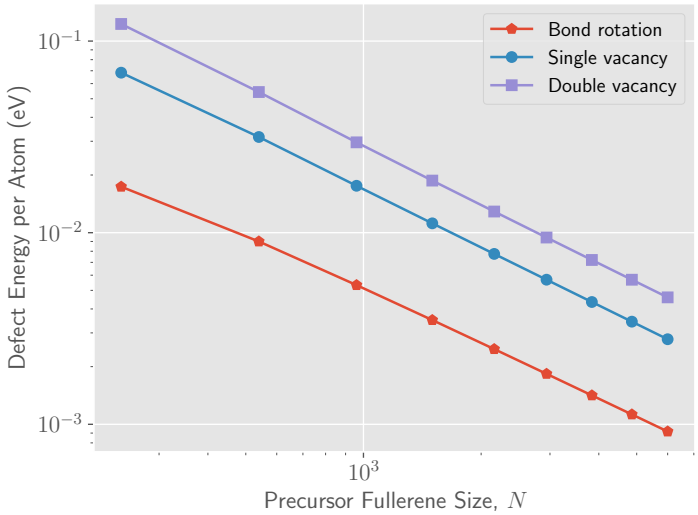

Figure A: Defect energy per atom for different defects introduced to icosahedral fullerenes as a function of the precursor size. The rotation of a bond (red pentagons) gives the smallest energy increase. In all three cases the effects of the defects decrease with increasing molecular size.

Per atom, the influences of the added defects are small, ranging from about 100 meV per atom for the double vacancy in the smallest fullerenes tested here (C_{240}), to energies on the order of 1 meV or less for fullerenes containing several thousand C atoms.