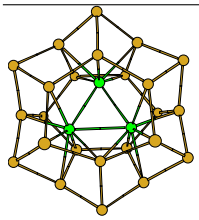
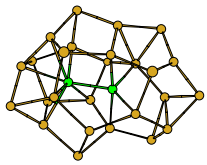
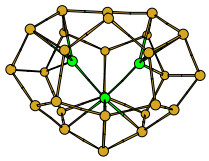
NTB Global-Minimum Clusters[a]



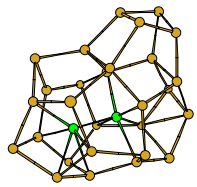
Si_{27}-ntb



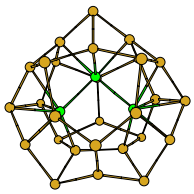
Si_{28}-ntb



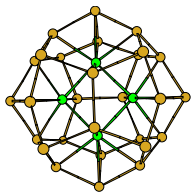
Si_{29}-ntb



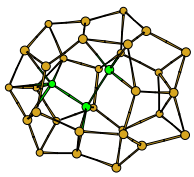
Si_{30}-ntb



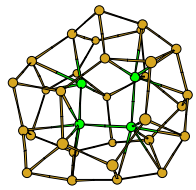
Si_{31}-ntb



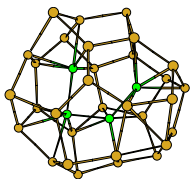
Si_{32}-ntb



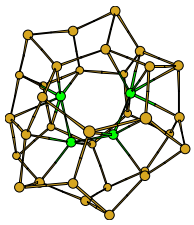
Si_{33}-ntb



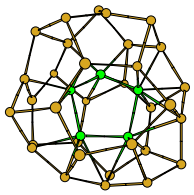
Si_{34}-ntb



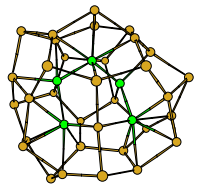
Si_{35}-ntb



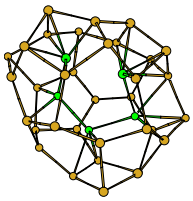
Si_{36}-ntb



Si_{37}-ntb



Si_{38}-ntb



Si_{39}-ntb

[a] Cluster coordinates will be post on The Cambridge Cluster Database (http://brian.ch.cam.uk/CCD.html).

Supporting FIG. 1. Yoo *et al*.

Supporting Table 1 Low-Lying Endohedral Silicon Fullerenes Optimized at B3LYP/6-31G(d) Level

	Single-point energy	BE/atom	ZPE	BE_total/atom
Si27	-7816.9365	3.321	0.0466	3.274
Si27a	-7816.9318	3.316	0.0469	3.269
Si28	-8106.4723	3.340	0.0494	3.292
Si29	-8395.9836	3.335	0.0508	3.287
Si29a	-8395.9733	3.325	0.0506	3.278
Si30	-8685.4995	3.334	0.0532	3.286
Si31	-8975.0395	3.355	0.0557	3.306
Si32	-9264.5479	3.347	0.0569	3.299
Si32a	-9264.5431	3.343	0.0571	3.294
Si33	-9554.0832	3.362	0.0592	3.313
Si34	-9843.5849	3.349	0.0606	3.301
Si35	-10133.1117	3.357	0.0631	3.308
Si36	-10422.6407	3.367	0.0645	3.318
Si37	-10712.1442	3.355	0.0670	3.306
Si38	-11001.6743	3.364	0.0686	3.315
Si39	-11291.1990	3.369	0.0701	3.320
Si25	-7237.9070	3.324	0.0437	**3.277**
Si33-Td	-9553.9526	3.254	0.0530	3.211
Si36-Cs	-10422.5716	3.313	0.0613	3.267
Si39-C3v	-11291.0814	3.287	0.0655	3.241

*Single-pointe energy = B3LYP/6-311G(2d) single-poing energy (hartree)
*BE/atom = B3LYP/6-311G(2d) binding energy (eV) /atom_number
*ZPE = zero-point correction (hartree) calculated at B3LYP/6-31G(d) level of theory
*BE_total/atom = [B3LYP/6-311G(2d) binding energy + ZPE] (eV)/atom_number

Supporting Table 2 NTB Global Minima Optimized at B3LYP/6-31G(d) Level

	B3LYP/6-311G(2d)	BE/atom
Si27ntb	-7816.9297	3.314
Si28ntb	-8106.4654	3.333
Si29ntb	-8395.9733	3.325
Si30ntb	-8685.4925	3.328
Si31ntb	-8975.0173	3.335
Si32ntb	-9264.5008	3.307
Si33ntb	-9554.0808	3.360
Si34ntb	-9843.5835	3.348
Si35ntb	-10133.0837	3.335
Si36ntb	-10422.6280	3.356
Si37ntb	-10712.1331	3.347
Si38ntb	-11001.6451	3.343
Si39ntb	-11291.1990	3.369