Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Structural growth pattern of neutral and negatively charged yttrium-doped silicon clusters $YSi_n^{0/-}$ (n=6-20): from linked to encapsulated structures

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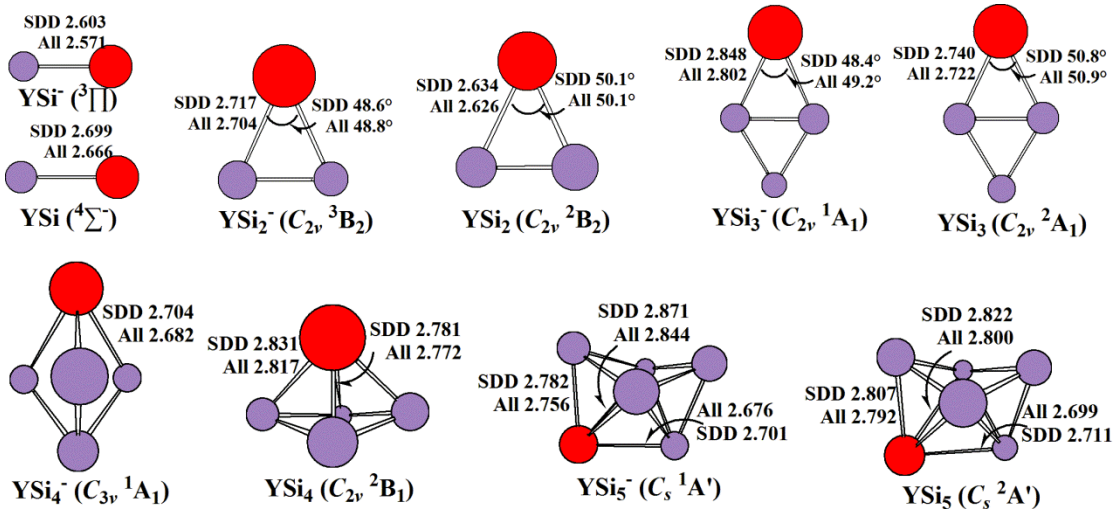

Figure S1. The ground state structures of neutral YSi_n (n=1-5) and their anions obtained at mPW2PLYP level. Bond distances are in Å. "SDD" indicates that the structural parameters are obtained with SDD basis set for Y atoms, while "All" indicates that the structural parameters are obtained with all-electron TZP basis set for Y atoms. The basis set for Si atoms is cc-pVTZ. The fifteen SDD Y-Si bond distances are averagely longer than those of all-electron TZP basis set by 0.021 Å.

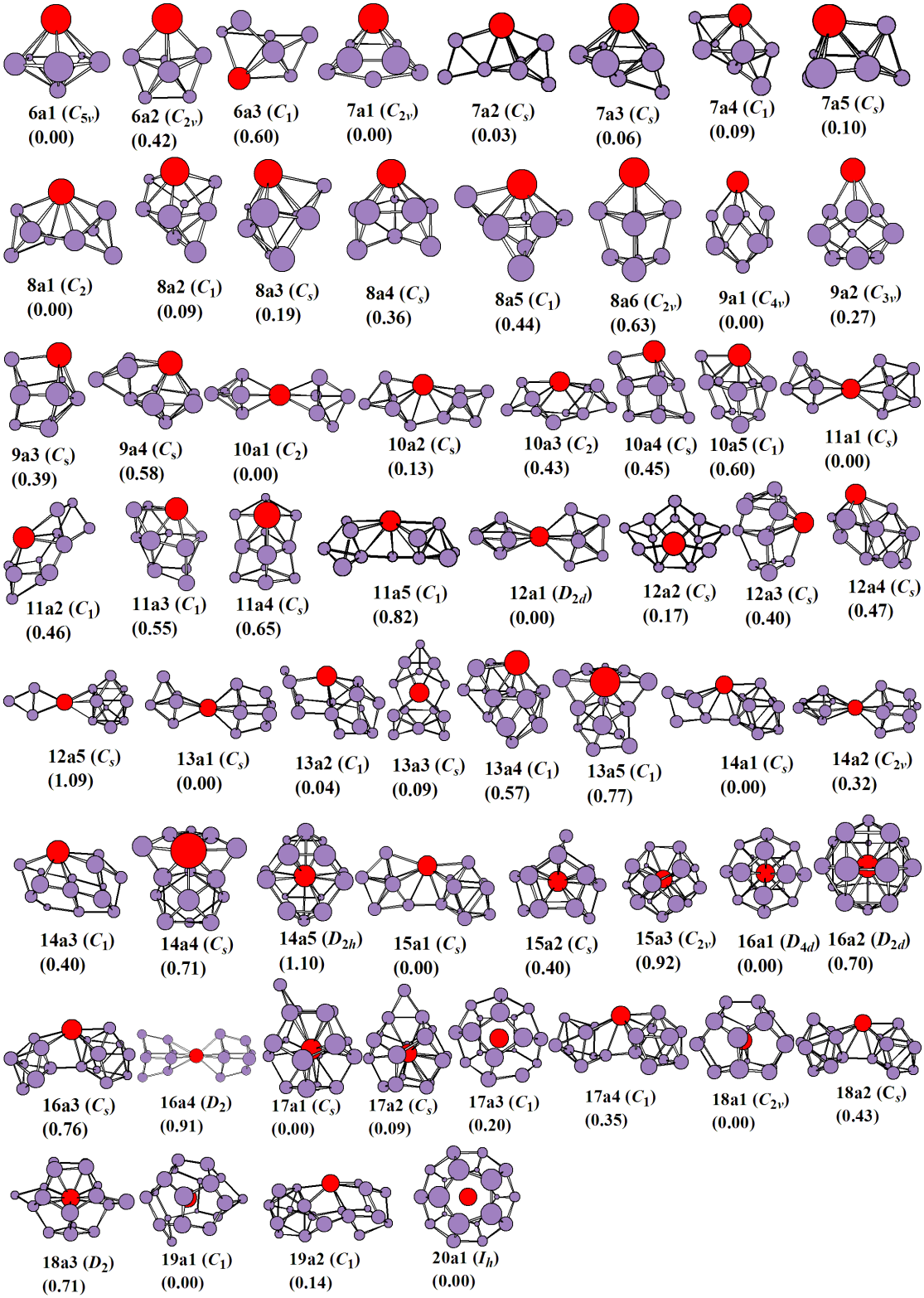

Figure S2. Low-lying isomers of anion YSi_n^- (n=6-20) clusters, point group and relative energy (in eV).

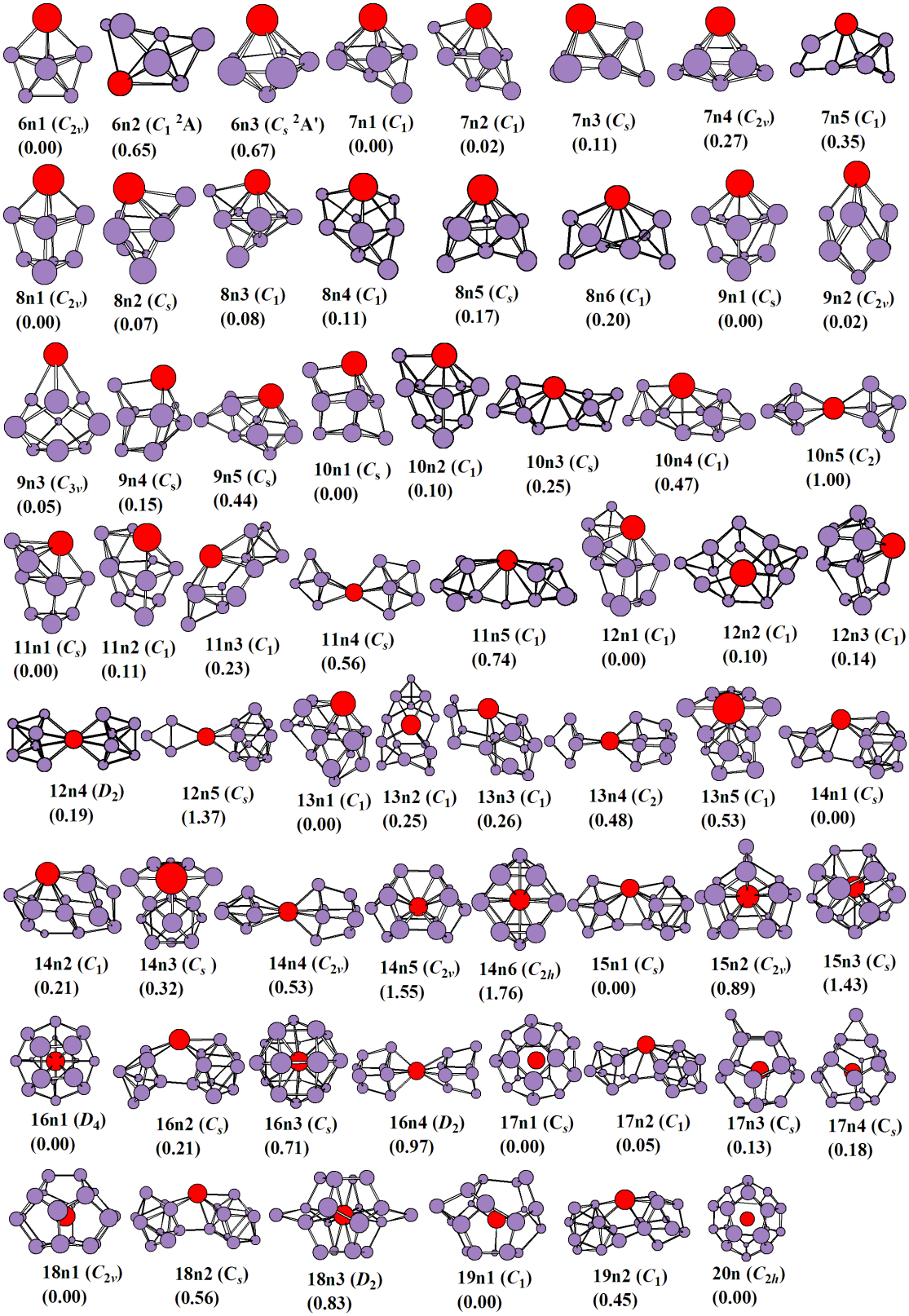

Figure S3. Low-lying isomers of neutral YSi_n (n=6-20) clusters, point group and relative energy (in eV).

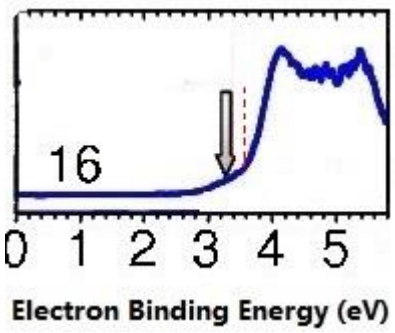

Figure S4. Photoelectron spectra of YSi_{16}^- taken from Reference 2. Black arrow pointed to the original AEA and red dashed line pointed to the new AEA.