Global minimum structures and electronic stability of Pt-doped silicon clusters $PtSi_n$ (n = 2 to 11) in neutral and anionic charge states
Electronic Supplementary Information

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1. xyz files

In this link

`https://doi.org/10.5281/zenodo.19357337`

the interested reader can download the xyz files of the local minima populations of the $PtSi_n$ (n = 2 – 11) clusters addressed in this investigation.

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2. Electrostatic potential surface peak values

Table S1: Peak values of $V_{S,\max}$ (kcal mol^{-1}) and FIA$^{\text{direct}}$ (kJ mol^{-1}) for the $PtSi_n$ series.

	$V_{S,\max}$	FIA$^{\text{direct}}$
$PtSi_2$	28.2	321.7
$PtSi_3$	29.0	361.8
$PtSi_4$	33.2	371.1
$PtSi_5$	20.7	330.9
$PtSi_6$	21.3	330.5
$PtSi_7$	25.7	367.7
$PtSi_8$	25.4	361.9
$PtSi_9$	28.9	381.5
$PtSi_{10}$	25.7	374.4
$PtSi_{11}$	23.2	372.3

3. Evolution of $V_{S,\mathrm{max}}$ and FIA$^{\mathrm{direct}}$

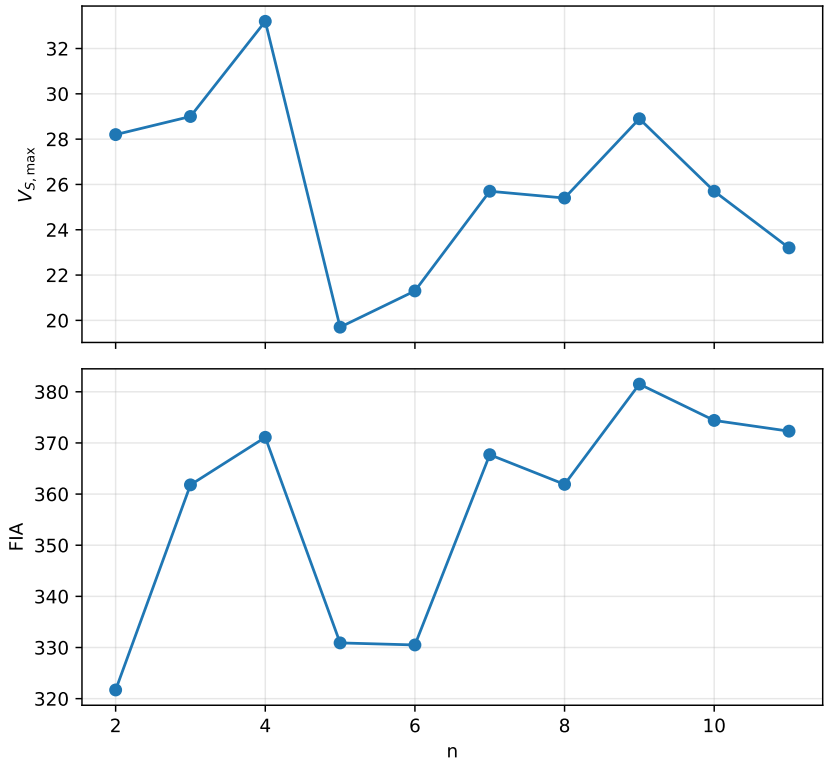

Figure S1: Size dependence of the maximum electrostatic potential on the van der Waals surface, $V_{S,\mathrm{max}}$ (top), and the fluoride ion affinity (FIA) (bottom) for $PtSi_n$ clusters as a function of n (n = 2 − 10).

4. Structures of the lowest-lying pure Silicon clusters and low-lying energy isomers of the $PtSi_n$ and $PtSi_n^-$ clusters

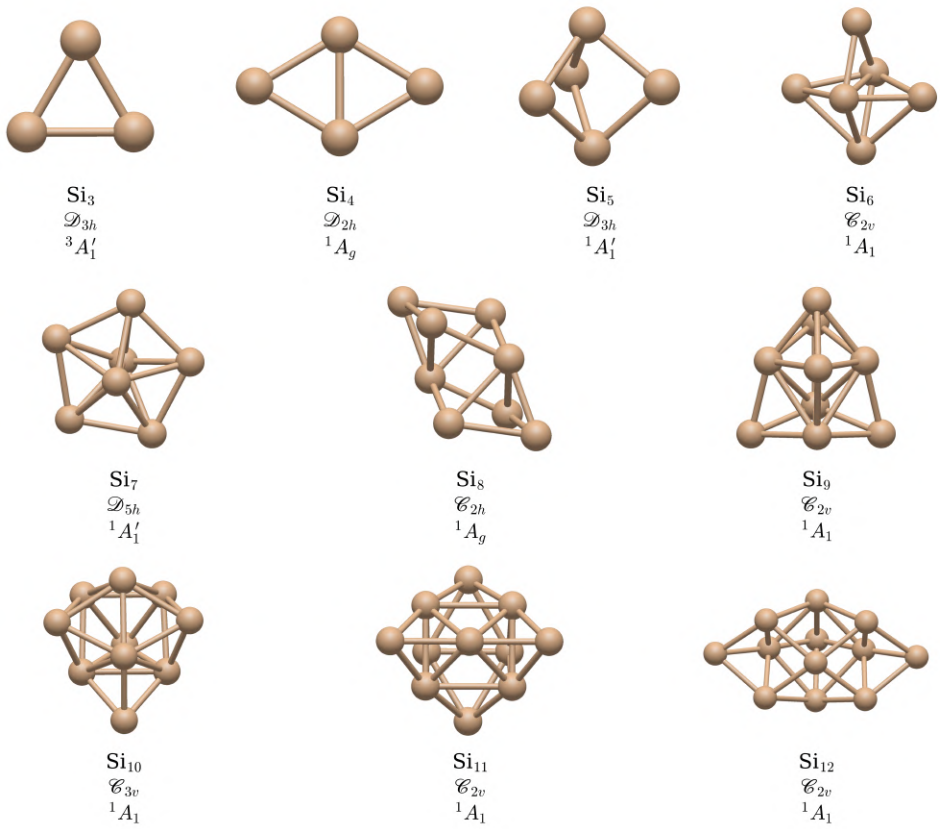

Figure S2: Lowest-lying energy isomers of the Si_n n = 3 − 12 clusters. The structures were taken from the Quantum Cluster Database (https://muellergroup.jhu.edu/qcd/).

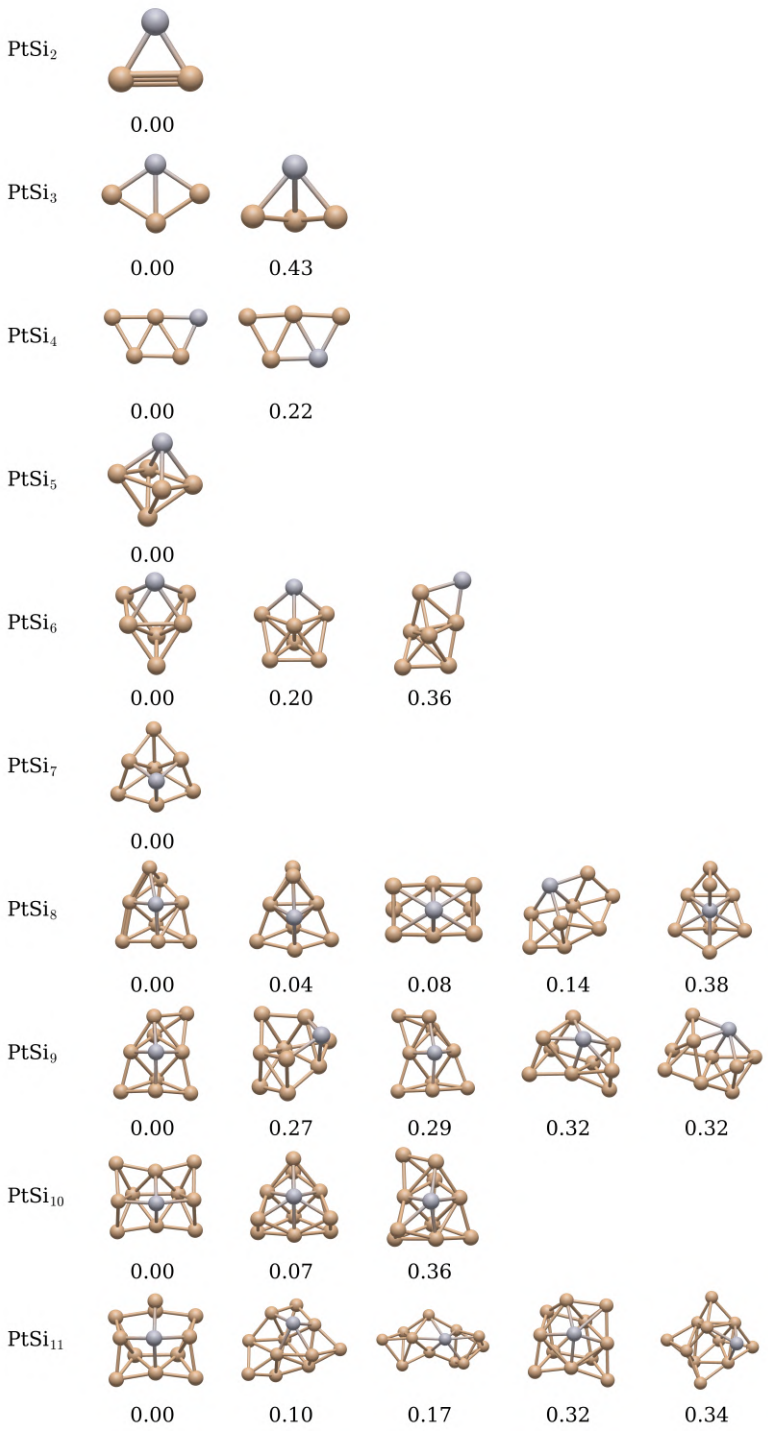

Figure S3: Low-lying energy isomers of the neutral $PtSi_n$ n = 2 – 11 clusters up to 0.5 eV. Relative energies in eV.

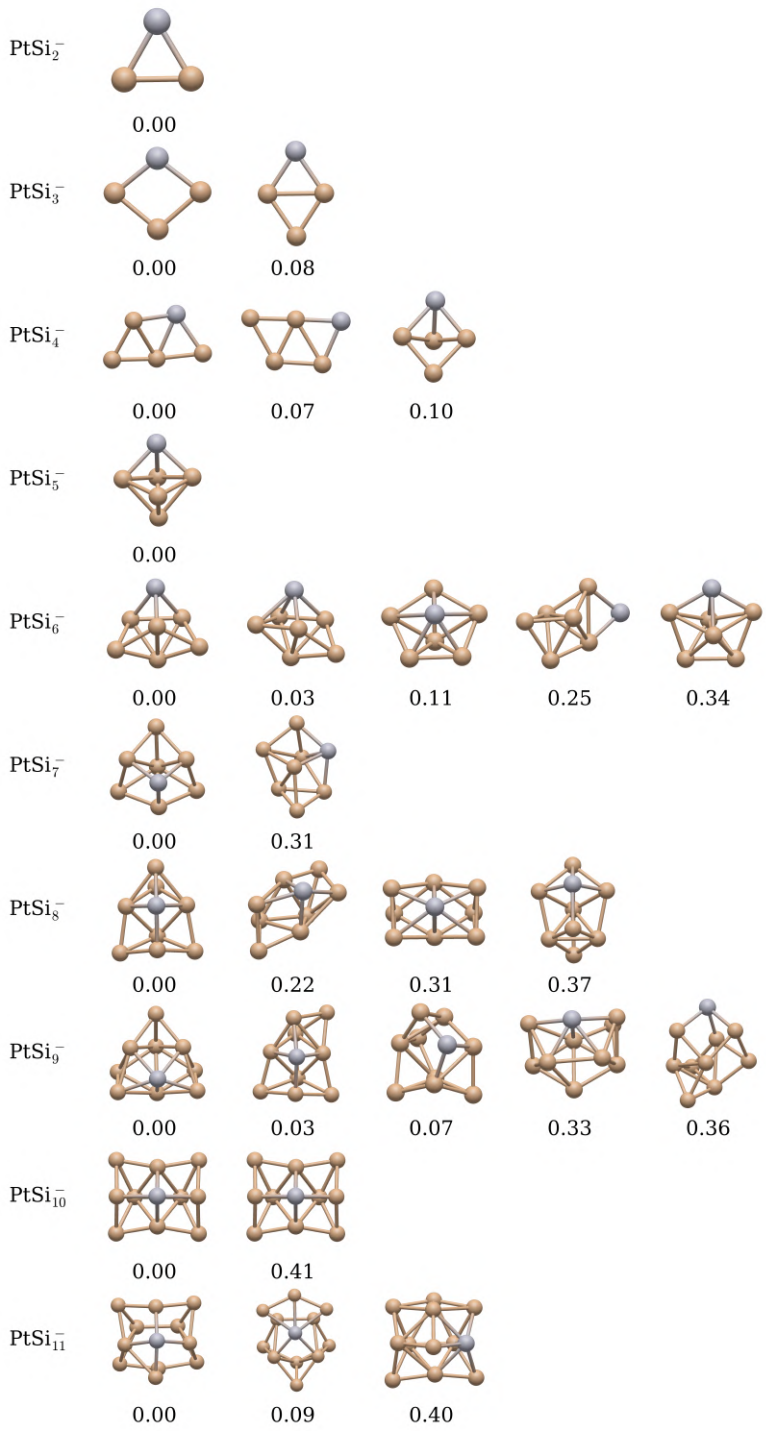

Figure S4: Low-lying energy isomers of the anionic $PtSi_n^-$ n = 2 – 11 clusters up to 0.5 eV. Relative energies in eV.

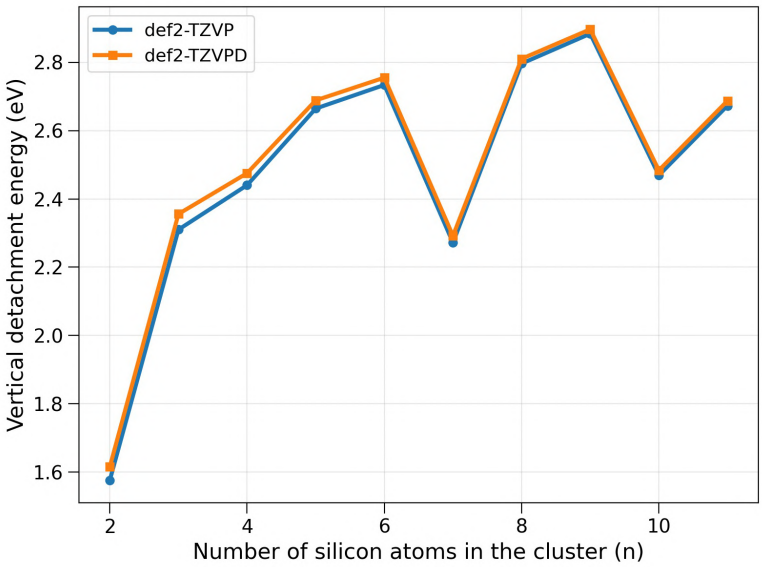

Figure S5: Vertical detachment energies for $PtSi_n^-$ clusters as a function of cluster size n, computed with the PBE0/def2-TZVP and PBE0/def2-TZVPD approximations.