# Electronic Supporting Information

## Electronic Structure and Thermochemical Properties of Silicon Doped Lithium Clusters $Li_nSi^{0/+}$, n = 1 – 8. New Insights on their Stability"

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**Table S1**. Total energies (a.u) of the low-lying isomers $Li_nSi^{0/+}$ with n = 1 ÷ 8 in both cationic and neutral states are obtained at the CCSD(T)/aVnZ (n = D, T, Q) levels and their CBS extrapolated energetic values.

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|---|---|---|
| $Li_2$ ($^1\sum_g^+$) | aVDZ | -14.90064 |
| | aVTZ | -14.90318 |
| | aVQZ | -14.90369 |
| | CBS | -14.90395 |
| $Si_2$ ($^3\sum_g^-$) | aVDZ | -577.93684 |
| | aVTZ | -577.98102 |
| | aVQZ | -577.99336 |
| | CBS | -578.00017 |
| $LiSi^+$ ($C_{\infty v}$, $^3\prod$) | aVDZ | -296.17892 |
| | aVTZ | -296.19626 |

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| | aVQZ | -296.20056 |
| | CBS | -296.20287 |
| LiSi ($C_{\infty v}$, $^4\sum^-$) | aVDZ | -296.41232 |
| | aVTZ | -296.43395 |
| | aVQZ | -296.43901 |
| | CBS | -296.44169 |
| $Li_2Si^+$ ($D_{\infty h}$, $^2\prod$) | aVDZ | -303.70776 |
| | aVTZ | -303.73417 |
| | aVQZ | -303.74052 |
| | CBS | -303.74389 |
| $Li_2Si$ ($D_{\infty h}$, $^3\sum^-_g$) | aVDZ | -303.89455 |
| | aVTZ | -303.92342 |
| | aVQZ | -303.93054 |
| | CBS | -303.93435 |
| $Li_3Si^+$ ($D_{3h}$, $^1A_1$') | aVDZ | -311.21454 |
| | aVTZ | -311.24752 |
| | aVQZ | -311.25566 |
| | CBS | -311.26002 |
| $Li_3Si$ ($C_{2v}$, $^2B_1$) | aVDZ | -311.38450 |
| | aVTZ | -311.41736 |
| | aVQZ | -311.42549 |
| | CBS | -311.42984 |
| $Li_4Si^+$ ($D_{4h}$, $^2A_{2u}$) | aVDZ | -318.72756 |

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| | aVTZ | -318.76446 |
| | aVQZ | -318.77371 |
| | CBS | -318.77869 |
| $Li_4Si$ ($C_{2v}$, $^1A_1$) | aVDZ | -318.88910 |
| | aVTZ | -318.92615 |
| | aVQZ | -318.93535 |
| | CBS | -318.94028 |
| $Li_5Si^+$ ($D_{3h}$, $^1A_1$') | aVDZ | -326.23724 |
| | aVTZ | -326.27838 |
| | aVQZ | -326.28889 |
| | CBS | -326.29458 |
| $Li_5Si$ ($C_{4v}$, $^2A_1$) | aVDZ | -326.37210 |
| | aVTZ | -326.41289 |
| | aVQZ | -326.42286 |
| | CBS | -326.42820 |
| $Li_6Si^+$ ($O_h$,$^2A_{1g}$) | aVDZ | -333.71648 |
| | aVTZ | -333.75974 |
| | aVQZ | -333.76998 |
| | CBS | -333.77540 |
| $Li_6Si$ ($O_h$,$^1A_{1g}$) | aVDZ | -333.85844 |
| | aVTZ | -333.90249 |
| | aVQZ | -333.91267 |

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|---|---|---|
| | CBS | -333.91803 |
| $Li_7Si^+$ ($C_{2v}$,$^1A_1$) | aVDZ | -341.18456 |
| | aVTZ | -341.22835 |
| | aVQZ | -341.23882 |
| | CBS | -341.24437 |
| $Li_7Si^+$ ($C_{3v}$, $^1A_1$) | aVDZ | -341.20044 |
| | aVTZ | -341.24601 |
| | aVQZ | -341.25692 |
| | CBS | -341.26272 |
| $Li_7Si^+$ ($C_{3v}$, $^1A_1$) | aVDZ | -341.19606 |
| | aVTZ | -341.24082 |
| | aVQZ | -341.25181 |
| | CBS | -341.25768 |
| $Li_7Si$ ($C_s$, $^2A'$) | aVDZ | -341.32520 |
| | aVTZ | -341.37071 |
| | aVQZ | -341.38163 |
| | CBS | -341.38744 |
| $Li_7Si$ ($C_{2v}$,$^2A_1$) | aVDZ | -341.31712 |
| | aVTZ | -341.36275 |
| | aVQZ | -341.37356 |
| | CBS | -341.37929 |
| $Li_8Si^+$ ($C_1$, $^2A$) | aVDZ | -348.65920 |
| | aVTZ | -348.70625 |

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|---|---|---|
| | aVQZ | -348.71746 |
| | CBS | -348.72341 |
| $Li_8Si^+$ ($D_{3d}$, $^2A_{2u}$) | aVDZ | -348.61407 |
| | aVTZ | -348.65916 |
| | aVQZ | -348.66971 |
| | CBS | -348.67527 |
| $Li_8Si$ ($C_2$, $^1A$) | aVDZ | -348.80728 |
| | aVTZ | -348.85467 |
| | aVQZ | -348.86587 |
| | CBS | -348.87179 |
| $Li_8Si$ ($C_{2v}$, $^1A_1$) | aVDZ | -348.79893 |
| | aVTZ | -348.84609 |
| | aVQZ | -348.85712 |
| | CBS | -348.86294 |
| $Li_8Si$ ($C_s$, $^1A'$) | aVDZ | -348.79925 |
| | aVTZ | -348.84687 |
| | aVQZ | -348.85798 |
| | CBS | -348.86384 |

**Figure S1**. The plot of density of states of $Li_5Si^+$ (**5c.1**) using orbitals obtained at the B3LYP/6-311+G(d) level

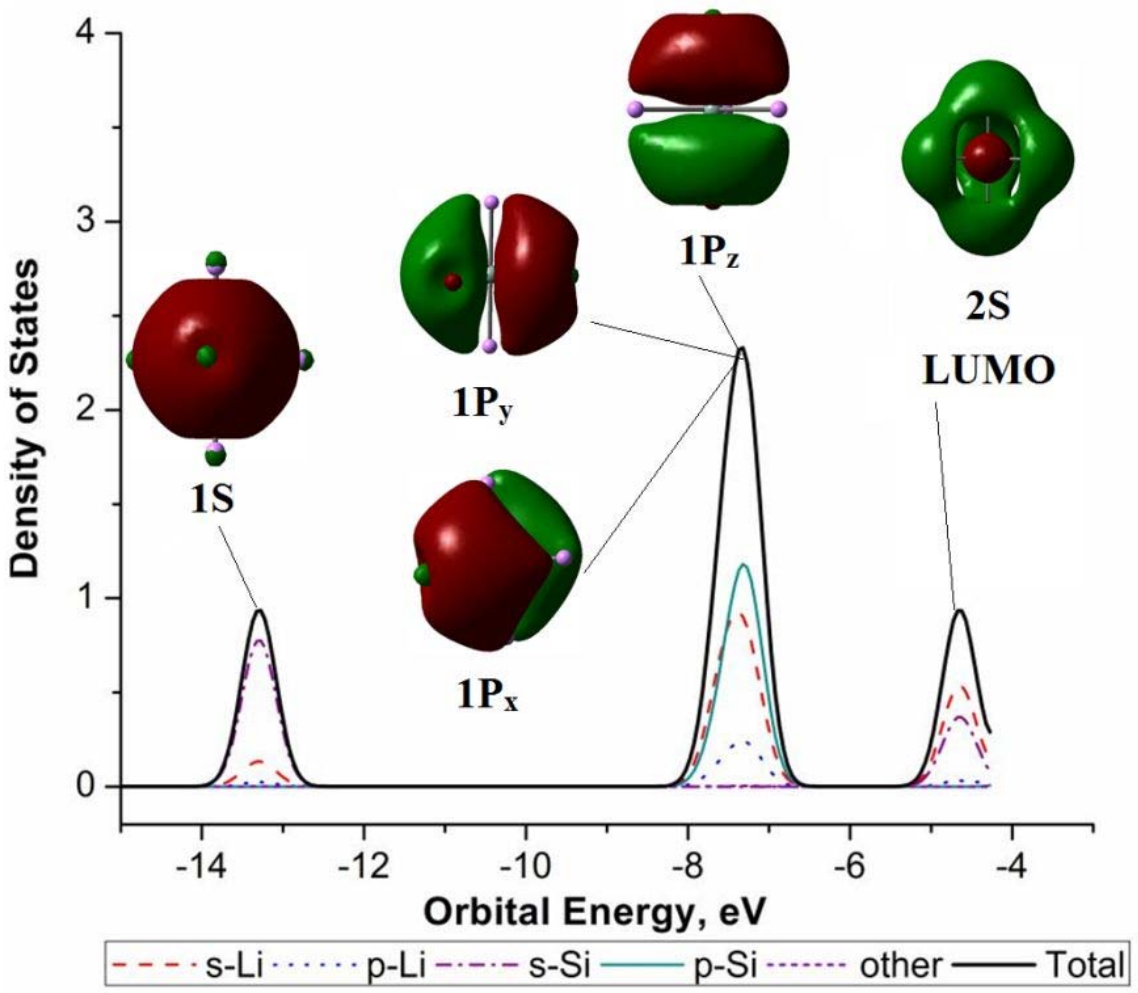

**Figure S2**. The plot of density of states of $Li_4Si$ (**4n.1**) using orbitals obtained at the B3LYP/6-311+G(d) level