

Supporting Information File

*Reexamination of the Origin of the Pseudo Jahn-Teller Puckering Instability
in Silicene*

Table S1 Standard errors for the fitting coefficients of the 4th order polynomial regression applied to the ground and excited states APES

Method	State	Standard errors*		
		a_0 (eV)	a_2 (eV/Å ²)	a_4 (eV/Å ⁴)
TPSSH	Ground	0.07	0.84	18.1
	1 B _{2g}	0.10	1.07	20.4
	2 B _{2g}	0.30	3.20	60.9
B3LYP	Ground	0.02	0.22	0.42
	1 B _{2g}	0.22	2.37	4.50
	2 B _{2g}	0.53	5.59	10.6

*All values must be multiplied by 10⁻²