

Supplemental Material on

# Graphitic phase of NaCl. Bulk properties and nanoscale stability

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**Table S1. Crystal data, density and bulk modulus for NaCl phases considered in this study**

Name	Pearson symbol	Space group	Coordinates	Lattice constants	V (Å <sup>3</sup> )	ρ (kg/cm <sup>3</sup> )	B <sub>0</sub> (GPa)
W		P63mc	$\frac{2}{3} \frac{1}{3} 0$ ; $\frac{1}{3} \frac{2}{3} \frac{1}{2}$ $\frac{2}{3} \frac{1}{3} u$ ; $\frac{1}{3} \frac{2}{3} \frac{1}{3} + u$ with $u \approx \frac{3}{8}$	a = 4.413 c = 10.850	30.530	1.589	17.04
B1		Fm-3m	0 0 0 $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	a = 5.687	23.011	2.109	24.72
B2		Pm-3m	0 0 0 $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	a = 3.500	21.456	2.262	26.20