Supplementary for "Direct and quasi-direct band gap silicon allotropes with remarkable stability"

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1. K-point mesh used in geometry optimizations and property investigations

Systems	Geometry optimization		property investigation	
	K-point mesh	Mesh space	K-point mesh	Mesh space
M585-silicon	3x9x6	0.0231,0.0291,0.0256	3x12x7	0.0231,0.0218,0.0219
S-silicon	9x2x5	0.0291,0.0291,0.0270	12x3x6	0.0217,0.0195,0.0225
Z-CACB-silicon	9x5x2	0.0291,0.0275,0.0287	12x7x3	0.0217,0.0196,0.0195
H-silicon	3x5x9	0.0282,0.0276,0.0292	4x7x12	0.0211, 0.0197, 0.0218
Z-CACB-silicon	5x9x3	0.0284,0.0292,0.0277	7x12x4	0.0202,0.0218,0.0208

2. Crystalline information for these new silicon allotropes:

H-silicon, Space group: PBAM (55); Lattice constants: a=11.831 Å, b=7.241 Å, c=3.810 Å, α=90°,β=90 °,γ=90 °

Four inequivalent atomic positions:

Si 1: 0.17603604, 0.97416948, 1.00000000

Si 2: 0.34456599, 0.80545555, 1.00000000

Si 3: 0.45548001, 0.85886885, 0.50000000

Si 4: 0.57373364, 0.60558225, 0.50000000

M585-silicon,Space group: P21/M(11); Lattice constants: a=14.643 Å, b=3.8137 Å, c=6.577 Å, α=90 °, β=81.53°, γ=90 °

Nine inequivalent atomic positions:

Si 1: 0.00228012, 0.25000000, 0.10542920

Si 2: 0.15274539, 0.25000000, 0.19078965

Si 3: 0.21320883, 0.75000000, 0.01197707

Si 4: 0.19477238, 0.25000000, 0.52000080

Si 5: 0.14621593, 0.75000000, 0.70911693

Si 6: 0.35790141, 0.25000000, 0.46354121

Si 7: 0.41679004, 0.75000000, 0.28463759

Si 8: 0.57820704, 0.75000000, 0.23080280

Si 9: 0.62700073, 0.25000000, 0.04153055

S-silicon, Space group: CMCM (63); Lattice constants: a=3.824 Å, b=17.135 Å, c=7.398 Å, α=90 °, β=90 °,γ=90 °

Four inequivalent atomic positions:

Si 1: 1.00000000, 0.05723600, 0.91332941

Si 2: 0.50000000, 0.13096622, 0.97907838

Si 3: 0.50000000, 0.22394755, 0.75000000

Si 4: 1.00000000, 0.30174630, 0.75000000

Z-ACA-silicon, Space group: PMMN (59); Lattice constants: a=7.051 Å, b=3.807 Å, 12.00 Å, $\alpha=90^{o}$, $\beta=90^{o}$, $\gamma=90^{o}$

Five inequivalent atomic positions:

Si 1: 0.50000000, 0.50000000, 0.95847243

Si 2: 0.00000000, 0.50000000, 0.93099914

Si 3: 0.73356913, 0.50000000, 0.82446719

Si 4: 0.67159392, 0.00000000, 0.71845391

Si 5: 0.81952057, 0.00000000, 0.54323041

Z-CACB-silicon, Space group: IMMA (74); Lattice constants: a=3.833 Å, b=7.285 Å, c=17.405 Å, $\alpha=90^{o}$, $\beta=90^{o}$, $\gamma=90^{o}$

Four inequivalent atomic positions:

Si 1:1.00000000, 0.41954631, 0.94159348

Si 2: 0.50000000, 0.49139768, 0.86979990

Si 3: 0.50000000, 0.75000000, 0.79039889

Si 4: 0.50000000, 0.25000000, 0.78605752