**Zeolite framework silicon allotropes with direct band gap**

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Table S1. The structural parameters of the new silicon allotropes

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| Structure | Wyckoff position |
| ACO | Si1: 16f (0.16000, -0.16000, 0.16000) |
| AEI | Si1: 16h (0.11507, -0.04262, 0.33406) |
|  | Si2: 16h (0.61319, -0.26326, -0.43848) |
| Si3: 16h (0.27489, -0.40488, 0.44662) |
| AFX | Si1: 24l (0.99807, 0.22648, 0.08053) |
|  | Si2: 24l (0.33484, 0.44070, 0.16905) |
| ANA | Si1: 48g (-1.12500, 0.15784, -0.09216) |
| BOZ | Si1: 16h (0.25732, -0.36622, -0.14207) |
|  | Si2: 16h (0.10476, -0.04163, -0.14126) |
| Si3: 16h (0.24545, -0.07851, -0.01285) |
| Si4: 16h (0.10525, -0.36601, -0.99072) |
| Si5: 8f (0.00000, -0.68267, -0.14153) |
| Si6: 8g (0.39466, -0.32089, -0.25000) |
| Si7: 4c (0.00000, -0.75187, -0.25000) |
| Si8: 8e (0.22315, 0.00000, 0.00000) |
| BPH | Si1: 12l (0.86441, 0.35154, 0.73930) |
|  | Si2: 12l (0.13542, 0.69175, 0.61885) |
| Si3: 4h (0.33333, 0.66667, 0.88252) |
| EDI | Si1: 4j (0.27997, 0.00000, 0.12472) |
|  | Si2: 1d (0.00000, 0.00000, 0.50000) |
| ETR | Si1: 12d (0.74463, 0.10733, 0.01595) |
|  | Si2: 12d (0.66790, 0.18737, 0.16048) |
| Si3: 12d (0.63517, 0.97157, 0.21897) |
| Si4: 12d (0.61013, 0.07651, 0.43260) |
| GME | Si1: 24l (0.43856, 0.10667, 0.09011) |
| LEV | Si1: 36i (0.99831, 0.23982, 0.06760) |
|  | Si2: 18g (0.23961, -0.00000, 0.50000) |
| LIT | Si1: 8d (-0.49425, 0.07153, 0.16069) |
|  | Si2: 8d (-0.32716, 0.57306, 0.67342) |
| Si3: 8d (-0.33447, 0.57312, 0.31725) |
| MEL | Si1: 16j (0.18924, 0.12267, -0.14384) |
|  | Si2: 16j (0.22128, 0.07697, -0.35650) |
| Si3: 16j (0.18849, 0.27861, -0.14100) |
| Si4: 16j (0.57727, 0.80883, -0.48988) |
| Si5: 16j (0.37667, 0.07752, -0.35359) |
| Si6: 8g (0.07770, 0.07770, 0.00000) |
| Si7: 8g (0.69177, 0.69176, -0.00000) |
| RWR | Si1: 16h (-0.00000, 0.30464, 0.17870) |
|  | Si2: 16g (0.70236, 0.70236, 1.00000) |
| SAT | Si1: 36i (-0.75620, -0.00171, -0.29414) |
|  | Si2: 36i (-0.57730, 0.33554, -0.21724) |
| SGT | Si1: 16h (-0.00000, 0.71354, 0.75450) |
|  | Si2: 16h (-0.00000, -0.14848, 0.67737) |
| Si3: 16h (-0.00000, -0.15269, 0.83578) |
| Si4: 16f (0.27722, -0.25000, 0.12500) |

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Figure S1. Phonon spectra for the zeolite framework silicon allotropes.

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Figure S2. Three-dimensional contour plots of electron effective masses for zeolite framework silicon allotropes with higher minimum electronic effective mass than diamond silicon.

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Figure S3. Three-dimensional contour plots of hole effective masses for zeolite framework silicon allotropes with higher minimum hole effective mass than diamond silicon.