

Supplementary Information for

From chemistry to mechanics: bulk modulus evolution of Li–Si and Li–Sn alloys via metallic electronegativity scale

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Table S1: Data for linear regression in Figure 1.

| Alloys | χ_A | χ_B | Z | V (Å ³) | B (GPa) |
|----------------------------------|----------|----------|----|---------------------|---------|
| Mg ₃ As ₂ | 1.25 | 2.31 | 16 | 1932.11 | 49.4 |
| MgAs ₄ | 1.25 | 2.31 | 4 | 481.57 | 43.4 |
| Mg ₂₃ Ba ₆ | 1.25 | 0.90 | 4 | 3525.69 | 24.4 |
| Mg ₂ Ba | 1.25 | 0.90 | 4 | 406.91 | 21.5 |
| Mg ₂ Ca | 1.25 | 1.02 | 4 | 339.69 | 30.1 |
| MgCd | 1.25 | 2.88 | 2 | 85.43 | 45.8 |
| MgCd ₃ | 1.25 | 2.88 | 2 | 172.98 | 48.2 |
| Mg ₃ Cd | 1.25 | 2.88 | 2 | 173.85 | 41.5 |
| MgCu ₂ | 1.25 | 4.26 | 8 | 352.64 | 88.6 |
| MgGa | 1.25 | 2.44 | 16 | 634.80 | 48.7 |

| | | | | | |
|---------------------------------|------|------|----|---------|--------|
| Mg ₂ Ga | 1.25 | 2.44 | 6 | 366.18 | 45.8 |
| Mg ₂ Ga ₅ | 1.25 | 2.44 | 4 | 546.43 | 52.4 |
| MgGa ₂ | 1.25 | 2.44 | 8 | 467.82 | 49.8 |
| Mg ₅ Ga ₂ | 1.25 | 2.44 | 4 | 583.05 | 43.9 |
| Mg ₂ Ge | 1.25 | 3.27 | 4 | 264.98 | 49.8 |
| MgLa | 1.25 | 1.60 | 1 | 62.38 | 34.1 |
| Mg ₂ La | 1.25 | 1.60 | 8 | 675.91 | 36 |
| Mg ₃ La | 1.25 | 1.60 | 4 | 421.88 | 37.2 |
| Mg ₂ Ni | 1.25 | 4.65 | 6 | 308.71 | 64.4 |
| MgNi ₂ | 1.25 | 4.65 | 8 | 317.66 | 123.2 |
| Mg ₂ Pb | 1.25 | 1.40 | 4 | 334.83 | 33.9 |
| Mg ₂ Si | 1.25 | 3.41 | 4 | 257.02 | 54.3 |
| Mg ₂ Sn | 1.25 | 2.86 | 4 | 317.91 | 40.5 |
| MgY | 1.25 | 1.67 | 1 | 55.00 | 41.1 |
| Mg ₂₄ Y ₅ | 1.25 | 1.67 | 2 | 1427.63 | 39.3 |
| AgMg | 3.77 | 1.25 | 1 | 37.06 | 63.76 |
| AgSc | 3.77 | 1.85 | 1 | 40.39 | 80.57 |
| AgZn | 3.77 | 3.22 | 1 | 31.52 | 99.2 |
| AgCd | 3.77 | 2.88 | 1 | 38.20 | 80.35 |
| AuMg | 3.78 | 1.25 | 1 | 36.33 | 82.92 |
| AuSc | 3.78 | 1.85 | 1 | 39.55 | 105.26 |
| AuZn | 3.78 | 3.22 | 1 | 32.13 | 122.2 |
| AuCd | 3.78 | 2.88 | 1 | 38.27 | 103.69 |
| MnRh | 4.58 | 4.31 | 1 | 24.24 | 178.9 |
| MnPd | 4.58 | 4.21 | 1 | 25.15 | 140.6 |
| MgZn ₂ | 1.25 | 3.22 | 4 | 203.15 | 64.66 |
| Mg ₄ Zn ₇ | 1.25 | 3.22 | 10 | 1896.47 | 59.12 |
| LiAl ₃ | 0.65 | 2.10 | 1 | 64.48 | 66.30 |
| Li ₂ Ca | 0.65 | 1.02 | 4 | 349.73 | 15.00 |
| LiAl | 0.65 | 2.10 | 8 | 249.45 | 47.80 |
| LiMg | 0.65 | 1.25 | 1 | 40.71 | 24.70 |
| Li ₃ Sb | 0.65 | 1.89 | 4 | 272.73 | 34.72 |
| Li ₃ Bi | 0.65 | 1.77 | 4 | 294.35 | 30.27 |
