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Thermoelectric Performance of ZrNX (X = Cl, Br, I) Monolayers

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Table S1. The optimized lattice constants (Å) and band gap (eV) of ZrNX monolayers calculated by the PBE functional with and without spin-orbit coupling (SOC). The relaxation condition of the maximum force on each atom is less than 0.01 eV/Å and 0.001 eV/Å were also tested.

		a	b	E_g
ZrNCl	0.01 eV/ Å, PAW	3.560	4.170	1.75
	0.001 eV/ Å, PAW	3.562	4.179	1.74
	0.001 eV/ Å, PAW+SOC	3.562	4.179	1.73
ZrNBr	0.01 eV/ Å, PAW	3.635	4.164	1.72
	0.001 eV/ Å, PAW	3.639	4.168	1.71
	0.001 eV/ Å, PAW+SOC	3.639	4.168	1.70
ZrNI	0.01 eV/ Å, PAW	3.760	4.160	1.28
	0.001 eV/ Å, PAW	3.774	4.165	1.28
	0.001 eV/ Å, PAW+SOC	3.774	4.165	1.16

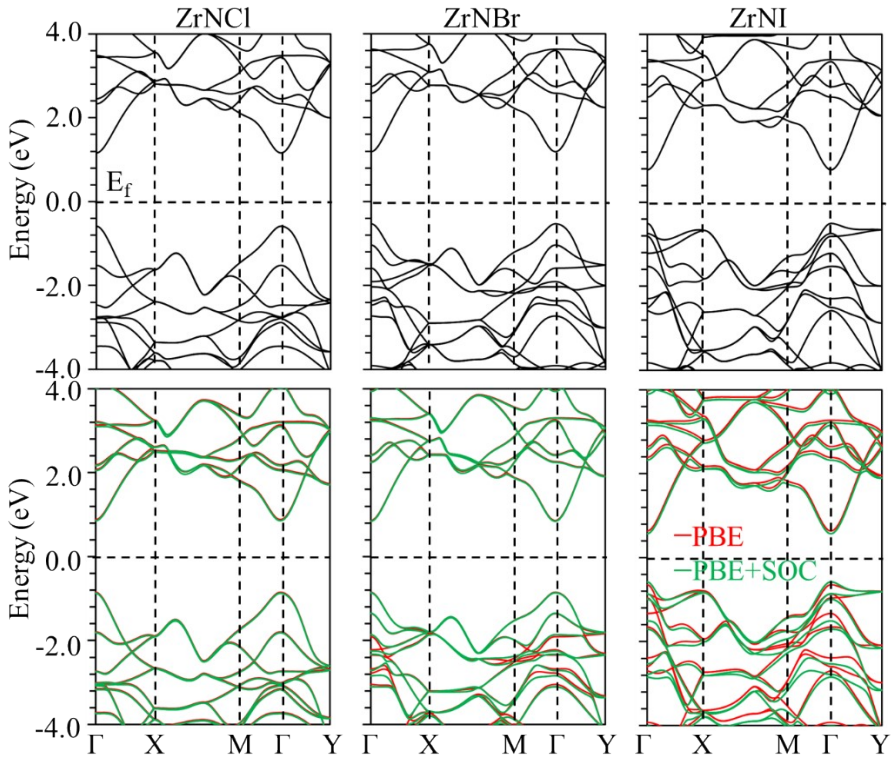

FIG. S1 Electronic band structures of ZrNX monolayers calculated by the PBE functional with spin-orbit coupling (SOC) (green lines) and without SOC (red lines). The Fermi energy level is set to zero. The SOC effect is negligibly affected the band structures of ZrNCl and ZrNBr monolayers. And the shape of the bands structure is not affected by the SOC effect in ZrNI monolayer, except for the 0.12 eV decreasing of the band gap. The top and bottom parts of figure are calculated with relaxation condition of the maximum force on each atom is less than 0.01 eV/Å and 0.001 eV/Å, respectively.

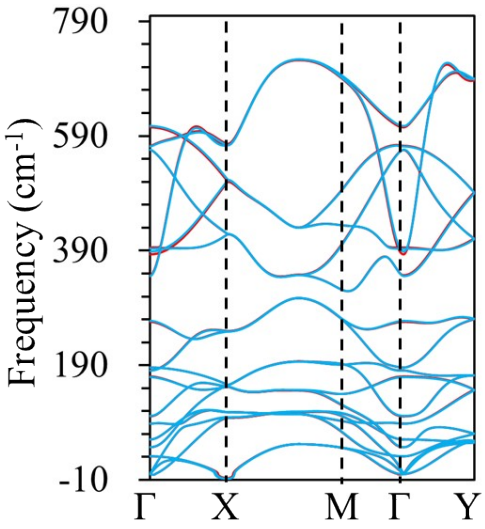

FIG. S2 Phonon dispersion structure of ZrNI monolayers along the highly symmetric k-point path in the first Brillouin zone (with VASP). The blue and red lines are calculated with relaxation condition of the maximum force on each atom is less than 0.01 eV/Å and 0.001 eV/Å, respectively.

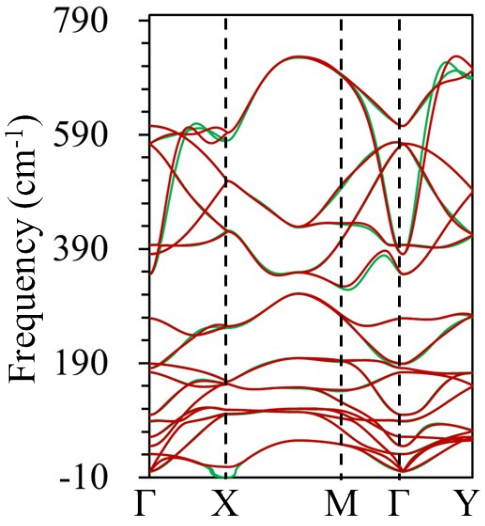

FIG. S3 Phonon dispersion structure of ZrNI monolayers along the highly symmetric k-point path in the first Brillouin zone (with PWmat). The green and red lines are calculated with a 5×5×1 supercell and a 6×5×1 supercell, respectively.

All the crystal structure and phonon spectrum calculations based on first principles, implemented in the PWmat package using GPU.[1] The Norm-Conserving Pseudopotential was used to describe the core-ion interactions, the generalized gradient approximations (GGA) of

the Perdew-Burke-Ernzerhof (PBE) functional is adopted for the exchange-correlation.[2, 3] A 70 Ry cutoff energy was used for the plane wave basis, and a 15 Å vacuum was adopted to avoid the fake interactions between the adjusts layers.

References

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