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In-plane Negative Poissons Ratios in 1T-Type Crystalline Two-Dimensional Transition Metal Dichalcogenides[1] LIPING YU, QIMIN YAN, ADRIENN RUZSINSZKY, Temple University — Materials with a negative Poissons ratio, also known as auxetics, exhibit counterintuitive mechanical behavior – becoming fatter when stretched and thinner when compressed. Such materials have enormous potential in many applications such as biomedicine and sensors but are exceedingly rare in nature. Despite that a variety of man-made auxetic materials have been discovered and fabricated, almost all of them are bulk materials with specially engineered porous structure with low density and stiffness. In this work, using first-principles calculations, we discover twelve single-layer two-dimensional transition metal dichalcogenides, MX_2 (M = Mo, W, Tc, Re; X = S, Se, Te), exhibiting intrinsic in-plane negative Poissons ratios in their 1T-type crystalline structure. The in-plane stiffness is predicted to be in the order of 10^2 GPa, at least three orders higher than most man-made auxetic materials. We attribute the occurrence of such auxetic behavior to the strong coupling between the chalcogen p orbitals and the intermetal t_{2g}-bonding orbitals within the basic triangular pyramid structure unit.

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