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First principles study on the atomic and electronic structures of stabilized atomic layer of transition metal[1] YOUNG JUN OH, KYEONGJAE CHO, Department of Materials Science and Engineering, The University of Texas at Dallas — Two-dimensional materials have gained a lot of attention due to their unique electronic properties and potential applications in electronic devices. Here, we perform first-principles calculations to investigate the stability and electronic structure of atomically thin transition metal layers. For 3d transition metal elements, silicene-like structure is the most stable among high symmetry structures that we considered. Calculated formation energy of thin transition metal layers is consistent with their tendency of melting temperature of bulk metals. For all transition metal elements, free-standing two-dimensional transition metal layers are found to be metallic. We discuss possible strategies to stabilize thin transition metal layers such as self-assembled monolayer or oxygen adsorption.

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