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Charge density wave metastability in Tantalum based transition metal dichalcogenide monolayers[1] DAVID MILLER, SUBHENDRA D. MAHANTI, PHIL DUXBURY, Department of Physics and Astronomy, Michigan State University — Understanding the interplay of charge density wave states, metal-insulator transitions and superconductivity in Tantalum based transition metal dichalcogenides is an important challenge for both theory and experiment. Depending on the choice of chalcogen; and the temperature, pressure and doping, different commensurate structures can occur. Using density functional theory we have studied the energetic stability of six different commensurate charge density wave structures in monolayer undoped TaX_2 for three chalcogens (X = S, Se, Te), providing an overview of low lying metastable structures that can occur in this family of materials.

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