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Origin of the Counterintuitive Dynamic Charge in the Transition-Metal Dichalcogenides[1] NICHOLAS PIKE, Université of Liège, BENOIT VAN TROEYE, Université Catholique de Louvain, ANTOINE DEWANDRE, Université of Liège, XAVIER GONZE, Université Catholique de Louvain, MATTHIEU VERSTRAETE, Université of Liège — Our recent first-principles calculations of the electronic and vibrational properties of the hexagonal transition-metal dichalcogenides reveal that their Born effective charges display a counterintuitive sign when compared to most other materials or transition-metal dichalcogenides with trigonal symmetry. We determine the origin of this counterintuitive sign by calculating the electronic, vibrational, and optical properties of these systems. We show that the sign of the Born effective charge is directly related to the electric field response of the electronic density, and, in turn, to the bonding characteristics of the material.There is a filled anti-bonding molecular orbital at the Fermi level, which is localized on the transition-metal atom and corresponds to a form of solid state π back-bonding in these material. We propose a method of determining if other materials display a similar counterintuitive sign, based on their bonding characteristics, and propose experiments which could measure the sign of the Born effective charge using different spectroscopies.

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