

First Principles Study of Helimagnetism in 1T-NiI₂ Monolayer

Juraj Mnich^{1, a)} and Martin Gmitra^{1, 2, b)}

¹*Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia*

²*Institute of Experimental Physics, Slovak Academy of Science, 04001 Košice, Slovakia*

^{a)} Corresponding author: juraj.mnich@student.upjs.sk

^{b)} martin.gmitra@upjs.sk

Abstract. Transition metal dihalide structures forming layered van der Waals materials exhibit often nontrivial magnetic order. Here studied 1T-NiI₂ belongs to the family of multiferroic dihalides with the helical magnetic ground state order. The helical state in monolayer 1T-NiI₂ differs from the cycloidal state in the bulk. Here we report that the ground state of 1T-NiI₂ monolayer is the proper helix, which is uniquely given by the propagation vector of the helix. The calculated in-plane ferroelectric polarization points perpendicularly to the helical propagation vector. The microscopic mechanism for the polarization is the p-d hybridization of the iodine p-orbitals and nickel d-orbitals.