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Hydrogen detection by a boron sheet: A theoretical study .[1] F. JAVIER DOMINGUEZ, Stony Brook University, MICHAL NOVOTNY, Comenius University, Bratislava, PREDRAG S. KRSTIC, Stony Brook University — A single boron sheet is now considered as a new nanomaterial with promising applications in electronics and as a sensor device. In this study we present quantum-classical molecular dynamic (QCMD) calculation of reflection, adsorption, and transmission processes of hydrogen impacting at energy in range 0.25 to 100 eV on a single boron sheet. Quantum-mechanical component of our QCMD approach is self-consistent charge tight binding density functional theory method (SCC-DFTB, [1]). We consider the corrugated boron sheet as our target, created experimentally [2], and compare our results with those reported for graphene [3], showing noticeable differences. [1] A. Mannix et al. Science 350, 1513 (2015). [2] M. Elstner et al. Phys. Rev. B 58, 7260 (1998) [3] R. C. Ehemann et al. Nanoscale research letter 7, 198 (2012)

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