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Electron Charge Transfer between Hydrogen Anions and Si Surfaces[1] BOYAN OBRESHKOV, UWE THUMM, Kansas State University — We show numerical results for the charge transfer between hydrogen anions and Si surfaces. The electronic structure of the substrate is derived from density functional theory with an application of the Thomas-Fermi-von Weizsäcker model extended to include linear and higher order non-linear dielectric response corrections to the kinetic energy density functional of non-interacting and non-uniform electron gas. An empirical local pseudopotential for Si [3] is used to represent the external field of the ionic cores of the substrate. The H^- neutralization probability near the surface is evaluated within a wave-packet propagation method for anions at grazing incidence with kinetic energy of 1 keV. We compare our theoretical negative-ion survival probabilities [1] with the experimental data in [2].

[1] B. Obreshkov, U. Thumm, Phys. Rev. A 74, 012901 (2006); and in preparation.
[2] M. Maazouz *et al.*, Surf. Sci. 398, 49 (1998).
[3] L. Wang and M. Teter, Phys. Rev. B 45, 13196 (1992).

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Boyan Obreshkov

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