

Abstract Submitted
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Stoichiometric anti-phase boundaries in monolayer boron-nitride¹

SIMONE S. ALEXANDRE, LIDIA C. GOMES, HELIO CHACHAM, RICARDO W. NUNES, U. F. Minas Gerais - Brazil — We propose a stoichiometric structure for domain boundaries in monolayer boron nitride, on the basis of the seeds of extended topological defect lines that have been observed in graphene under electronic irradiation [1]. The structure consists of a periodic extended line defect with an atomic structure consisting of alternating fourfold and eightfold BN rings. The structure is shown to be lower in energy than non-stoichiometric counterparts, and to lead to the formation of shallow electron and hole bands inside the band gap of the BN bulk matrix. We suggest that the existence of such defect bands may be experimentally observed in optical experiments.

[1] J. Kotakoski, A. V. Krasheninnikov, and J. C. Mayer, Physical Review Letters, 106, 105505 (2011).

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Simone S. Alexandre
U. F. Minas Gerais - Brazil

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