Abstract Submitted
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Superconducting transition temperature of a boron nitride layer with a high niobium coverage.[1] GERARDO VAZQUEZ, FERNANDO MAGANA, Instituto de Fisica, UNAM — We explore the possibility of inducing superconductivity in a Boron Nitride (BN) sheet, by doping its surface with Nb atoms sitting on the center of the hexagons. We used first-principles density functional theory in the general gradient approximation. The Quantum-Espresso package [1] was used with norm conserving pseudo potentials. The structure considered was relaxed to their minimum energy configuration. Phonon frequencies were calculated using the linear-response technique on several phonon wave-vector meshes. The electron-phonon coupling parameter was calculated for a number of k meshes. The superconducting critical temperature was estimated using the Allen-Dynes formula with $\mu^* = 0.1$ - 0.15. We note that Nb is a good candidate material to show a superconductor transition for the BN-metal system. [1] Giannozzi P, Baroni S, Bonini N, Calandra M, Car R, Cavazzoni C, *et al.* Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials. J Phys Condens Matter 2009; 21**:** 395502-19.

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