Abstract Submitted
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**Superconductivity near structural phase transition: the case of NbN**[1] SIMON BLACKBURN, MICHEL CÔTÉ, Département de physique, Regroupement québécois des matériaux de pointe (RQMP), Université de Montréal, Canada, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, University of California at Berkeley and Materials Sciences Division of Lawrence Berkeley National Laboratory — Using density functional theory within the local density approximation we report the study of the electron-phonon coupling in $NbC_{1-x}N_x$ crystals in the rocksalt structure. The Fermi surface of the system allows important nesting. The associated Kohn's anomaly greatly increases the electron-phonon coupling and induces a structural instability when the electronic density of states reaches a critical value. Our results reproduce the observed rise in $T_c$ from 11.2 K to 17.3 K as the nitrogen doping is increased. To further understand the important effect of the structural instability to the superconducting temperature, we model the Eliashberg spectral function with two contributions, one for the unstable phonons and the other for the unaffected phonons. Using the McMillan formula, we can predict the evolution of $T_c$ within this simple model that reproduces well our *ab initio* results and the experimental data.

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