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Exchange and correlation effects on the superconducting transition of two-dimensional multivalley semiconductors[1] BETUL PAMUK, CNRS and Université Pierre et Marie Curie, JACOPO BAIMA, ROBERTO DOVESI, Università di Toriono, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université Pierre et Marie Curie — It has recently been shown that the enhancement in the superconducting temperature of two-dimensional semiconductors at low doping is linked to the electron-electron interaction enhancing the response to the valley polarization that is due to the electron-phonon coupling [1]. In this work, we extend this study to analyze the exchange and correlation effects on the electronic, magnetic, and vibrational properties of Li-doped ZrNCl and HfNCl - typical examples of two-dimensional two-valley semiconductors. We show that these properties can be calculated by *ab initio* density functional theory only by using approximations beyond the generalized gradient approximation. Finally, we present the link between the enhancement of the spin susceptibility and superconducting temperature by demonstrating that the electron-phonon coupling is acting as a pseudo-magnetic field causing the valley polarization. [2] [1] M. Calandra, P. Zoccante and F. Mauri, Phys. Rev. Lett. **114**, 077001 (2015) [2] B. Pamuk *et al.*, in preparation

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