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Ab initio molecular dynamics simulations of electron doped ZrNCl ANTIA S. BOTANA, FRANCOIS GYGI, WARREN E. PICKETT, University of California Davis — When electron doped, the layered transition metal nitride ZrNCl becomes superconducting with an impressive critical temperature T_c= 15K. Its isovalent sisters become superconducting at 17K (TiNCl) and 26K (HfNCl). This class has very strong 2D character, as cuprates, iron pnictides, and MgB_2, but the pairing interaction is not magnetic nor conventional electron-phonon in origin. To explore the dynamical behavior of electrons doped into a highly ionic insulator, ab initio molecular dynamics calculations have been carried out on doped ZrNCl. The simulations allow us to analyze the electronic response in real space, and to study the differences in behavior of the two experimental mechanisms of doping electronic carriers: alkali metal intercalation and Cl vacancies, both of which give nearly the same high critical temperature.

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