

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Superconducting properties in  $\text{Li}_x\text{ZrNCl}$  from first principles**

PAOLO ZOCCANTE, Université P. et M. Curie, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université P. et M. Curie —  $\text{ZrNCl}$  is a layered band insulator. Upon Li intercalation it undergoes a metal-superconductor transition at 5% Li content. The superconducting critical temperature displays a very peculiar behaviour as it is maximal ( $T_C = 15.2\text{K}$ ) for  $\approx 5\%$  intercalation, at the edge of the insulator-superconductor transition. When the Li concentration is increased the critical temperature decreases monotonically, stabilizing at  $T_C = 11.5\text{K}$  for  $x=0.3$ . We present calculations beyond DFT on  $\text{Li}_x\text{ZrNCl}$  as a function of doping. We show that an ultradense sampling of the Brillouin zone (both for phonon and electron momentum) is necessary to describe the phonon spectra and the electron-phonon coupling in this material. We show that marked Kohn-anomalies, overlooked in all previous calculations, occur in the phonon spectrum at different energy scales. Finally, we discuss the role of correlation effects in determining the superconducting properties of  $\text{Li}_x\text{ZrNCl}$ .

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Date submitted: 13 Nov 2013

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