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Unified picture of the doping dependence of superconducting transition temperatures in alkali metal/ammonia intercalated FeSe DANIEL GUTERDING, HARALD JESCHKE, Institute for Theoretical Physics, University of Frankfurt, Frankfurt a.M., Germany, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL, ROSER VALENTI, Institute for Theoretical Physics, University of Frankfurt, Frankfurt a.M., Germany
— We present a theoretical investigation of alkali metal/ammonia intercalated iron selenide [1]. Using ab-initio density functional theory we unravel how charge doping and dimensionality of the electronic structure can be controlled through the chemical composition of the intercalated molecules. Within random phase approximation spin fluctuation theory we analyze the impact of intercalation on the superconducting pairing strength. We find that high T_c is to be expected away from perfect nesting. While experimental studies have focused on the intercalation of larger molecules in the spacer layer so far, we argue that no higher T_c can be achieved this way. This work was supported by Deutsche Forschungsgemeinschaft under Grant No. SPP 1458, the National Science Foundation under Grant No. PHY11-25915 and the Department of Energy under Grant No. DE-FG02-05ER46236.

[1] D. Guterding et al., arXiv:1410.7565

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