Abstract Submitted
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Towards a quantitative description of tunneling conductance of superconductors ANDREAS KREISEL, ITP, U. Leipzig, Germany, R. NELSON, RWTH Aachen University, Germany, T. BERLIJN, CNMS, Oak Ridge Nat. Lab., USA, W. KU, Dept. of Phys. and Astr., Shanghai Jiao Tong U., China, R. ALURU, P. WAHL, H. ZHOU, SUPA, U. St. Andrews, UK, U.R. SINGH, MPI-FKF, Stuttgart, Germany, S. CHI, R. LIANG, W.N. HARDY, D.A. BONN, Dept. of Phys. and Astr., UBC, Canada, P.J. HIRSCHFELD, Dept. of Physics, U. Florida, USA, B.M. ANDERSEN, NBI, U. Copenhagen, Denmark — Since the discovery of iron-based superconductors, a number of theories have been put forward to explain the qualitative origin of pairing, but there have been few attempts to make quantitative, material-specific comparisons to experimental results. We use first principles electronic structure calculations to make predictions for the superconducting gap and calculate the surface wavefunctions within the same framework. We present a detailed comparison between theory and scanning tunneling experiments for the material LiFeAs, where nonpolar surfaces have allowed collection of very high resolution data[1]. For the homogeneous system we find that the calculated topographic images show a transition between registered As and Li lattices as a function of set-point bias as it is also seen experimentally[2]. We show further that generic weak to intermediate strength impurity potentials lead to resonances tied to the lower gap edge, and discuss conclusions that can be drawn about the superconducting order parameter from these observations. [1] S. Chi, et al., Phys. Rev. B 94, 134515 (2016) [2] A. Kreisel, et al., arXiv:1610.00619

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