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Anisotropic Migdal-Eliashberg theory using Wannier functions¹ ELENA ROXANA MARGINE, FELICIANO GIUSTINO, University of Oxford — We combine the fully anisotropic Migdal-Eliashberg theory with electron-phonon interpolation based on maximally-localized Wannier functions, in order to perform reliable and highly accurate calculations of the anisotropic temperature-dependent superconducting gap and critical temperature of conventional superconductors. Compared with the widely used McMillan approximation, our methodology yields a more comprehensive and detailed description of superconducting properties, and is especially relevant for the study of layered or low-dimensional systems as well as systems with complex Fermi surfaces. In order to validate our method, implemented within the EPW package [1,2], we perform calculations on two prototypical superconductors, Pb and MgB₂, and obtain good agreement with previous studies [3]. [1] F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007). [2] J. Noffsinger et. al., Computer Physics Communications 181, 2140 (2010). [3] E. R. Margine and F. Giustino, Phys. Rev. B (submitted).

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