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**Electron transport calculations with Wannier functions in van der Waals heterostructures** WUSHI DONG, ALEJANDRO LOPEZ-BEZANILLA, PETER LITTLEWOOD, University of Chicago, Argonne National Laboratory, ANDREAS ROELOFS' GROUP AT ARGONNE NATIONAL LAB COLLABORATION — The vertical stacking of 2D materials forming van der Waals heterostructures (vdWHs) exhibits a wide range of interesting properties. A combined approach based on the Green's function formalism and a mean-field description of the electronic structure is used to calculate vertical electron transport in vdWHs. Tight-binding parameters obtained from Maximally Localized Wannier Functions enable us to model quantum electron transport at low computational costs. Our analysis of electron transport efficiencies provides the foundation and motivation for experimental works.

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