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Quantitative bond energetics in atomic-scale junctions with significant van der Waals character LATHA VENKATARAMAN, Columbia Univ, SRIHARSHA ARADHYA[1], Columbia University, Applied Physics, MARK HYBERTSEN, CFN, Brookhaven National Labs, — A direct measurement of the potential energy surface that characterizes individual chemical bonds in complex materials has fundamental significance for many disciplines. Here, we demonstrate that the energy profile for metallic single-atom contacts and single-molecule junctions can be mapped by fitting ambient atomic force microscope measurements carried out in the near-equilibrium regime to a physical, but simple, functional form.[1] In particular we are able to extract bond energies for metal-molecule link bonds in cases where the interaction has significant contribution from nonspecific interactions attributed to van der Waals (vdW) interactions at short length scale in addition to specific donor-acceptor bonds.[2] Our approach significantly expands the quantitative information extracted from these measurements, allowing direct comparisons to density functional theory (DFT) calculations instead of relying on trends in bond rupture forces alone. [1] S.V. Aradhya, A. Nielsen, M.S. Hybertsen, L. Venkataraman, ACS Nano 8, 7522–7530 (2014) [2] S.V. Aradhya, M. Frei, M.S. Hybertsen, L. Venkataraman, Nature Materials, 11, 872-876, (2012)

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