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Abstract for an Invited Paper
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Functional Theories of Heat and Charge Transport¹

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I will discuss non-equilibrium density functional theories of local temperatures and associated heat and charge currents that are particularly suited for the study of thermoelectric phenomena. In one case, I will introduce a functional theory of open quantum systems [1] that allows for the study of local temperatures by the introduction of local thermal probes. In another [2], we couple the local temperature field to an energy density operator. I will also provide predictions on the local temperature oscillations in atomic wires [3], carbon nano-ribbons and graphene junctions [4], and discuss similarities and differences between the different local temperature definitions in the strongly-correlated regime [5]. Work supported by DOE. [1] M. Di Ventra and R. D' Agosta, Phys. Rev. Lett. 98, 226403 (2007). [2] F. Eich, G. Vignale and M. Di Ventra, Phys. Rev. Lett. 112, 196401 (2014). [3] Y. Dubi and M. Di Ventra, Nano Lett. 9, 97 (2008). [4] J.P. Bergfield, M. A. Ratner, C. A. Stafford, and M. Di Ventra, Phys. Rev. B 91, 125407 (2015). [5] L.Z. Ye, D. Hou, X. Zheng, Y.J. Yan, and M. Di Ventra, Phys. Rev. B 91, 205106 (2015).

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