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**Towards ab-initio device-level electronic structure models with Density Functional Theory**

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Density functional theory has been the champion of electronic structure of molecules and materials in the past 40 years. Despite such a success story, issues linger. Among them, the cubic computational scaling with increasing system size and the need to compute a large number of bands when metals and semiconductors are considered. These issues are cutting short DFT's applicability to materials science and engineering. In my talk, I will show how density embedding [1] coupled with orbital-free DFT [2,3] can radically change this outlook. Finite size effects become inessential when metals and nanoparticles are treated at the orbital-free DFT level [4] and molecules and low-dimensionality periodic materials are treated at the Kohn-Sham DFT level. Accuracy remains the same as regular DFT because of a new generation of functionals improves dramatically the applicability of orbital-free DFT. The talk concludes with a brief venture in the nonequilibrium state of materials [5] discussing opportunities for multiscale ab-initio models and how those can be translated into force fields of broad applicability. References [1] W. Mi and M. Pavanello, J. Phys. Chem. Lett., **11** 272 (2020) [2] W. Mi and M. Pavanello, Phys. Rev. B, **100**, 041105 (2019) [3] W. Mi, A. Genova, and M. Pavanello, J. Chem. Phys., **148**, 184107 (2018) [4] X. Shao, K. Jiang, W. Mi, A. Genova and M. Pavanello, WIREs: Comp. Mol. Sci., ASAP (2020)