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**Stationary state Kohn-Sham Theory: Modern algorithms breathe new life into an old theory** DENIZ GUNCELER, RAVISHANKAR SUNDARARAMAN, T.A. ARIAS, Cornell University — In this talk, we will discuss stationary-state Kohn-Sham theory, an old (Phys. Rev. B 31, 6264-6272) but largely ignored idea that is recently undergoing revival. It is based on an in-principle exact scheme in which excited states are computed as the stationary states of the Hohenberg-Kohn functional. We will discuss the objections of Gaudoin and Burke (Phys. Rev. Lett. 93, 17), and also describe the computational difficulties which prevented this theory from becoming popular in the past, and present new algorithms for computing the predictions of this theory. The resulting technique has inherent computational advantages over TDDFT and GW, and results using semilocal functionals show great promise for molecules. However, the method as implemented exhibits large errors for solids. In this talk, we shall show that the origin of this behaviour is related to the fact that different errors dominate the solid and molecular cases, and we shall discuss prospects for improvement of the theory in the future.

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