A constraint method for variational total energy calculations of electronic excitations within the Kohn-Sham scheme\textsuperscript{1} BABAK SADIGH, Lawrence Livermore National Laboratory — We propose a general constraint on the occupations of single-particle orbitals within (hybrid) density-functional theory that allows a variational total energy formulation for extended systems containing arbitrary electronic excitations. This method is simple to implement and is ideal for studying structural relaxations and molecular-dynamics simulations in the presence of excitations since accurate forces can be calculated via the Hellman-Feynman theorem.

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