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Pressure Dependent Electronic Properties of Organic Semiconductors from First Principles FRANZ KNUTH, CHRISTIAN CARBOGNO, Fritz-Haber-Institut der MPG, Berlin, DE, VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, DE; Duke University, Durham, NC, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress, and pressure [1]. In this contribution, we present the theoretical background, assessment of approximations, and results of electronic and transport properties in the framework of density-functional theory. Our implementation considers the analytical strain derivatives (stress tensor) including the contributions that stem from (a) van-der-Waals interactions [2] and (b) the Fock-exchange in hybrid functionals. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene and anthracene under hydrostatic pressure. We show that the fraction of exact exchange included in the calculations is critical – and non-trivial to choose – for a correct description of these systems. Furthermore, we point out trends for the electrical conductivity under pressure and identify the dominant charge carriers and transport directions.

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