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Density Functional Methods and Electronic Processes in Organic Materials[1] QIN WU, Brookhaven National Lab — When modeling the fundamental processes in organic electronic materials, ab initio calculations play an important role because they provide an independent source of information. It is thus critical to use accurate and reliable ab initio methods. In this talk, we will share our experience in using density functional methods to study charge generation and transport in some organic systems. These include prototypical polythiophene and polyfluorene, as well as some newly synthesized conjugated molecules. They all have strong dispersion forces and strong electron-vibration coupling; both are well-known difficult effects for density functional methods to capture accurately. We will describe our effort in exploring ways to do meaningful calculations. Close collaborations with experimental work will also be emphasized.

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