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Theoretical insights into multiscale electronic processes in organic photovoltaics SERGEI TRETIAK, Los Alamos Natl Lab — Present day electronic devices are enabled by design and implementation of precise interfaces that control the flow of charge carriers. This requires robust and predictive multiscale approaches for theoretical description of underlining complex phenomena. Combined with thorough experimental studies such approaches provide a reliable estimate of physical properties of nanostructured materials and enable a rational design of devices. From this perspective I will discuss first principle modeling of small-molecule bulk-heterojunction organic solar cells and push-pull chromophores for tunable-color organic light emitters. The emphasis is on electronic processes involving intra- and intermolecular energy or charge transfer driven by strong electron-phonon coupling inherent to pi-conjugated systems. Finally I will describe how precise manipulation and control of organic-organic interfaces in a photovoltaic device can increase its power conversion efficiency by 2-5 times in a model bilayer system. Applications of these design principles to practical architectures like bulk heterojunction devices lead to an enhancement in power conversion efficiency from 4.0% to 7.0%. These interface manipulation strategies are universally applicable to any donor-acceptor interface, making them both fundamentally interesting and technologically important for achieving high efficiency organic electronic devices.

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