Cracking the atomic mystery of perovskite solar cell materials with neutron scattering

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Perovskite $CH_3NH_3PbI_3$ exhibits outstanding photovoltaic performances, but the understanding of the atomic motions remains inadequate even though they take a fundamental role in transport properties. Here, we present a complete atomic dynamic picture consisting of molecular jumping rotational modes and phonons, which is established by carrying out high-resolution time-of-flight quasi-elastic and inelastic neutron scattering measurements in a wide energy window ranging from 0.0036 to 54 meV on a large single crystal sample, respectively. The ultrafast orientational disorder of molecular dipoles, activated at ~165 K, acts as an additional scattering source for optical phonons as well as for charge carriers. It is revealed that acoustic phonons dominate the thermal transport, rather than optical phonons due to sub-picosecond lifetimes. These microscopic insights provide a solid standing point, on which perovskite solar cells can be understood more accurately and their performances are perhaps further optimized.