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**Theoretical Studies of Carrier Diffusion in Perovskite Tantalum Oxynitride Photocatalyst** HIROKI IRIGUCHI, ERIKO WATANABE, KOICHI YAMASHITA, Univ. of Tokyo — Water-splitting photocatalysts have been attracting considerable attention in the scientific community since they enable to produce clean and environmentally friendly chemical energy in the form of H<sub>2</sub>. Perovskite BaTaO<sub>2</sub>N (BTON) is expected to be a performing photocatalyst due to its band structure suitable for visible light absorption and overall water-splitting reaction. Indeed, successful hydrogen evolution and oxygen evolution reactions are reported under sacrificial reagent. However, to achieve highly efficient overall water-splitting, electronic properties such as carrier diffusion are need to be improved. In our study, we investigate the carrier diffusion properties in BTON by focusing on cooling process of hot carriers via phonon, by means of first-principles calculations combining Density Functional Theory (DFT) and Many-body Perturbation Theory (MBPT). In particular, we calculated the lifetime of hot carrier in BTON by evaluating electron-phonon coupling constant. We found that BTON has very short carrier lifetime with an order of 1 fs. We also clarified that anion ordering, i.e. the anionic distribution of O<sup>2-</sup> and N<sup>3-</sup> in the oxynitride, affects the lifetime of hot hole.

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