Abstract Submitted
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Tempo-spatially resolved dynamics of elec- trons and holes in bilayer MoS2-WS2[1] J.M. GALICIA-HERNANDEZ, University of Puebla, Puebla 72550, Mexico and University of Central Florida, Orlando, FL 32816, V. TURKOWSKI, University of Central Florida, Orlando, FL 32816, G. HERNANDEZ-COCOLETZI, University of Puebla, Puebla 72550, Mexico, T.S. RAHMAN, University of Central Florida, Orlando, FL 32816 — We have performed a Density-Matrix Time-Dependent Density-Functional Theory analysis of the response of bilayer MoS2-WS2 to external laser-pulse perturbations. Time-resolved study of the dynamics of electrons and holes, including formation and dissociation of strongly-bound intra- and inter-layer excitonic states, shows that the experimentally observed [1] ultrafast inter-layer MoS2 to WS2 migration of holes may be attributed to unusually large delocalization of the hole state which extends far into the inter-layer region. We also argue that the velocity of the hole transfer may be further enhanced by its interaction with transfer phonon modes. We analyze other possible consequences of the hole delocalization in the system, including reduction of the effects of the electron-electron and hole-hole repulsion in the trions and biexcitons as compared to that in the monolayers. [1] X. Hong et al., Nature Nano 9, 682 (2014).

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