Coherent phonons and polarons in efficient bioi nanoplatelet photocatalysts

Sebastian Rieger1, Killian Frank2, Bert Nickel2, Tim Fürmann1, Jochen Feldmann1, Jacek K. Stolarczyk1,3,\*

# 1Chair for Photonics and Optoelectronics, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstraße 10, 80539 Munich, Germany

# 2Department of Physics and CeNS, Ludwig-Maximilians-Universiät München, Geschwister-Scholl-Platz 1, 80539 Munich, Germany

# 3Instytut Fizyki im. M. Smoluchowskiego, Uniwersytet Jagielloński, ul. Łojasiewicza 11, 30‑348 Kraków, Poland

\*autor korespondencyjny: jacek.stolarczyk@uj.edu.pl

 Applications of semiconductors in photocatalysis rely on efficient separation of the photoinduced charge carriers. An elegant way to achieve this without complicated device architectures is by using anisotropic nanocrystals capable of inherent charge carrier separation, without the need of an interface. Bismuth oxyhalides (BiOX, X = Cl, Br, I) are an emergent family of promising photocatalysts for hydrogen generation that consist of oppositely charged layers in the crystal structure.

We show that the excitation of 3-15 nm thin BiOI nanoplatelets by a femtosecond laser pulse creates coherent phonons that cause a time-variant modulation of the optical density in a form of a damped temporal oscillation. This is consistent with the presence of a built-in dipolar electric field and its sub-picosecond screening by the photoexcited charge carriers. The detected phonon modes correspond exclusively to vibronic motion normal to the layers implying ultrafast charge separation between the oppositely charged layers.

We further demonstrate that the strong electron phonon-coupling results, once the initially coherent phonons dephase, in the self-trapping of the carriers within separate layers and the formation of polarons. This inhibits carrier recombination and provides them with the opportunity to reach the catalytically active sites and efficiently drive surface photocatalytic reactions. This shows that inherent anisotropy of BiOI is a critical factor for its photocatalytic activity.