# Single-layer Group-IVB nitride halides as promising photocatalysts

Jian Liu[1,2,3], Xi-Bo Li[1], Da Wang[1], Hao Liu[4], Ping Peng*[2], Li-Min Liu*[1]

[1]*Beijing Computational Science Research Center, Beijing 100084, China*
[2]*School of MaterialsScience& Engineering,Hunan University, Changsha 410082, Hunan, China*
[3]*College of Electrical & Information Engineering, Hunan Institute of Engineering, Xiangtan 411105, Hunan, China*
[4]*Chengdu Green Energy and Green Manufacturing Technology R&D Center, Chengdu, Sichuan, 610207, China*

**Corresponding author: limin.liu@csrc.ac.cn, ppeng@hnu.edu.cn*

*Table S1 The calculated lattice constants of bulk β-form MNX with PBE functional with or without vdW correction compared with experimental results.*

| | PBE | | PBE+ vdw-optB88 | | Experiment | |
|---|---|---|---|---|---|---|
| | a | c | a | c | a | c |
| ZrNCl | 3.647 | 28.694 | 3.642 | 27.730 | 3.605 | 27.672[1] |
| ZrNBr | 3.682 | 30.341 | 3.676 | 29.465 | 3.640 | 29.270[2] |
| ZrNI | 3.758 | 32.509 | 3.756 | 31.729 | 3.718 | 31.381[2] |
| HfNCl | 3.589 | 28.517 | 3.580 | 27.643 | 3.577 | 27.711[1] |
| HfNBr | 3.628 | 31.377 | 3.618 | 29.430 | 3.610 | 29.294[2] |
| HfNI | 3.710 | 36.136 | 3.703 | 31.666 | 3.689 | 31.329[2] |

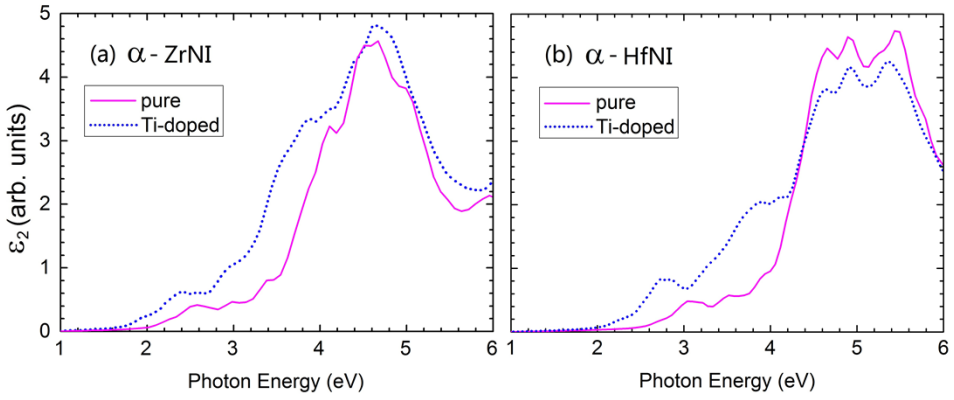


*Fig.S1 Imaginary part of the dielectric function, $\varepsilon_2$, as a function of photon energy $\hbar\omega$ for (a) pure and 12.5% Ti-doped single-layer α-ZrNI and (b) pure and 12.5% Ti-doped single-layer α-HfNI. $\varepsilon_2$ is calculated using the PBE functional followed by a rigid energy shift to take into account the bandgap underestimation of the PBE functional.*

1. X. Chen, T. Koiwasaki and S. Yamanaka, *Journal of Solid State Chemistry*, 2001, **159**, 80-86.
2. X. Chen, H. Fukuoka and S. Yamanaka, *Journal of Solid State Chemistry*, 2002, **163**, 77-83.