Abstract Submitted
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The first-principles study on the electronic and optical properties of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ from many-body perturbation theory HIROKI KAWAI, GIACOMO GIORGI, The University of Tokyo, MAURIZIA PALUMMO, The University of Rome "Tor Vergata", KOICHI YAMASHITA, The University of Tokyo — Gallium zinc oxynitride $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ is one of the promising candidates as overall water-splitting photocatalyst under visible light. In 2005, the high photocatalytic activity was reported on the GaN-rich alloys[1] and nowadays, the ZnO-rich ones with the higher visible-light absorption were also synthesized by some groups[2, 3]. Thus the further improvement of the photocatalytic water splitting is being expected. In spite of such a huge potential of this material, the origin of the visible-light absorption is not well understood. The first-principles methods based on many-body perturbation theory (MBPT), GW approximation and Bethe-Salpether equation, combining with density functional theory, enable us to do reliable analysis of the electronic and optical properties. On this meeting, we will discuss the origin of visible-light absorption of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ by MBPT results focusing on the non-isovalent character. [1]K. Maeda. et al. *J.Am.Chem.Soc.* 127, 8286 (2005), [2]H. Chen. et al. *J.Phys.Chem.C*, 114, 1809 (2010), [3]K. Lee. et al. *Nano Lett*, 12, 3268 (2012)

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