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Electronic structures and optical properties of GaN and ZnO nanowires T. AKIYAMA, A.J. FREEMAN, Northwestern U., K. NAKAMURA, T. ITO, Mie U., Japan — GaN and ZnO are promising semiconductor materials that exhibit many outstanding physical and chemical properties. Recently, their one-dimensional nanowires (NWs) are also attracting much interest due to their significant potential for optoelectronic nano-devices [1]; they always take the wurtizte structure while other compound semiconductor NWs also exhibit other polytypes [2]. However, little is known about their electronic and optical properties. Here we investigate the electronic structures and optical properties of GaN and ZnO [0001] NWs by using the highly precise full-potential linearized augmented plane wave (FLAPW) method [3]. Our calculations demonstrate that the band gap energy of both the unpassivated and passivated NWs becomes large compared with the bulk energy gap due to quantum confinement effects; surface states crucially affect the electronic structure of unpassivated NWs. Further, we find peculiar features of their dielectric functions that exhibit strong anisotropy in the calculated optical properties. Work supported by the U.S. NSF (through its MRSEC Program at NU).

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Toru Akiyama
Northwestern University

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