Cavity space changes insulator to metal
- Elucidation of origin of metallic electronic structure of Na_3N -

Inorganic clathrates have provided a platform for rich intercalation chemistry and have been used widely in application. Among these, the inner cavity space rarely affects the electronic structure of the framework. We report that the anti-ReO_3-type compound Na_3N has a metallic nature irrespective of the stoichiometric chemical composition of simple representative elements and that this unusual nature originates from the collapse of the bandgap owing to the presence of a crystallographic cavity. We synthesized Na_3N by the plasma-assisted nitridation of alkali metals, and diffuse reflectance measurements indicated a metallic nature. The crystallographic cavity in the nitride interacted with Na and N to modify the electronic structure, resulting in the collapse of the bandgap. Na_3N is a unique nitride, which possesses an electronically active cavity space.