

NRC主催／物理工学コース／談話会

平成29年2月6日（月）16:00～17:00

総合研究棟W棟 7階 W701 演習室

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The Modulation of Nearly Free Electron States in MXenes by Electric Fields: A First-Principles Study

As new members of two-dimensional family, the transition metal carbides (namely MXenes) and their functionalized derivatives, exhibit many different physical and chemical properties. Recently, based on the density functional theory, we have reported the nearly free electron (NFE) states in different MXenes functionalized by -OH (Phys. Rev. B 93, 205125). Most of these MXene monolayers are metallic, but $\text{Sc}_2\text{C}(\text{OH})_2$ and $\text{Y}_2\text{C}(\text{OH})_2$ are semiconductors. As the further study, we find that their conduction bands, stemming from the NFE, are not far away from their Fermi levels and can be modulated by the external electric fields. As the results, their band gaps can be engineered. The manipulation of gap width indicates that they can be used as electric devices.

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