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TiC2: A New Two-Dimensional Sheet beyond MXenes TIANSHAN ZHAO, Virginia Commonwealth Univ, SHUNHONG ZHANG, YAGUANG GUO, QIAN WANG, peking university — MXenes are attracting attention due to their rich chemistry and intriguing properties. Here a new type of metal-carbon-based sheet composed of transition metal centers and C2 dimers rather than individual C atoms is designed. Taking the Ti system as a test case, density functional theory calculations combined with a thermodynamic analysis uncover the thermal and dynamic stability of the sheet, as well as a metallic band structure, anisotropic Young's modulus and Poisson's ratio, a high heat capacity, and a large Debye stiffness. Moreover, the TiC2 sheet has excellent Li storage capacity with a small migration barrier, a lower mass density compared with standard MXenes, and better chemical stability as compared to the MXene Ti2C sheet. When Ti is replaced with other transition metal centers, diverse new MC2 sheets containing C=C dimers can be formed, the properties of which merit further investigation.

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