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Correction: Investigations of the structural, electronic, and optical properties of Ti_3XC_2 (X = Ge, Pb, or Bi) by DFT

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Correction for 'Investigations of the structural, electronic, and optical properties of Ti_3XC_2 (X = Ge, Pb, or Bi) by DFT' by Haider Hussain *et al.*, *Phys. Chem. Chem. Phys.*, 2026, https://doi.org/10.1039/d4cp04277h.

In the originating article, the material was misclassified as an MXene. This led to an inaccurate description of the material throughout the text. This misclassification does not affect the computational findings regarding the structural, electronic, and optical properties of Ti_3XC_2 (X = Ge, Pb, or Bi). However, the interpretation of its potential applications reflects MAX-phase characteristics rather than MXene properties. Specifically, the retention of the "A" layer implies differences in electronic behavior, surface chemistry, and exfoliation potential.

The manuscript introduction is updated to introduce the material correctly:

Introduction

The global transition toward renewable energy has significantly increased the demand for advanced functional materials capable of supporting next-generation energy storage and electronic technologies. Conventional technologies, such as lithium-ion batteries and vanadium redox flow batteries, rely heavily on transition metals like cobalt and nickel. Although these materials provide reasonable performance, their widespread application is limited by environmental concerns, resource scarcity, and energy-intensive production processes. To address these challenges, researchers are increasingly exploring alternative materials composed of earth-abundant elements that can deliver comparable or superior performance while minimizing ecological impact.

MAX phases represent a promising class of layered materials with the general formula $M_{n+1}AX_n$, where M is an early transition metal, A is an A-group element, and X is carbon or nitrogen. These materials exhibit a unique combination of metallic and ceramic properties. MAX phases, comprising alternately stacked transition metal (M), A-group element (A), and carbon/nitrogen (X) layers, are stabilized by robust M–X bonds and comparatively weaker M–A interactions. Targeted removal of the A-layer enables the formation of two-dimensional Ti_3C_2 MXenes, illustrating the intrinsic structural tunability of these layered systems.[1,2] The feasibility of exfoliation depends on the bonding strength between the M and A layers in the parent MAX phase, making an understanding of A-site chemistry essential for evaluating both intrinsic structural properties and the potential suitability of these materials for electrochemical applications.

Previous theoretical and experimental studies have investigated the stability and electronic structure of Ti_3AC_2 (A = Al, Si, Sn) MAX phases. The stability of these materials has been attributed primarily to strong Ti–C bonding interactions mediated by Ti 3d electrons.[3] Substitution of different A-site elements significantly influences the structural and mechanical characteristics of the material. For instance, variations in atomic size among A-site elements affect lattice parameters and interlayer bonding strength.[4,5] Larger atoms such as Ge tend to increase the *c*-axis lattice parameter and reduce Ti–A bond stiffness, thereby modifying the structural characteristics of the layered framework. Differences in atomic radius can also influence the electronic structure of the material, as observed in comparative studies involving Si, Ge, and Sn substitutions.[6]

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Further studies have demonstrated that compositional variations within MAX phases can lead to notable differences in mechanical behavior. For example, Ti_3CdC_2 has been reported to exhibit a brittle nature, whereas Ti_3PC_2 shows relatively ductile characteristics.[7] Electrical resistivity calculations for compounds such as Ti_2AlC, Ti_3AlC_2, and Ti_3SiC_2 have also revealed that MAX phases typically exhibit metallic conductivity due to the presence of Ti 3d electronic states near the Fermi level.[8] In addition, strong Ti–C bonding has been identified as a key factor contributing to the structural stability of these compounds.[9,10]

Among larger A-site elements, Ti_3GeC_2 has often been reported to exhibit relatively high structural stability within the MAX-phase family. However, previous theoretical investigations indicate that Ti_3AlC_2 possesses a lower formation energy, indicating that it is thermodynamically easier to form during synthesis.[11] This observation reveals that formation energy primarily determines the thermodynamic feasibility of synthesis, whereas structural stability may also depend on bonding strength and lattice configuration after formation.

Although extensive research has been conducted on the structural and electronic properties of MAX phases, comparatively fewer studies have focused on their optical characteristics. Optical investigations of Ti_3GeC_2 and Ti_3SiC_2 have revealed significant reflectivity, slow light propagation, and pronounced energy-loss features associated with their layered metallic electronic structures.[12] Similarly, Ti_3AlC_2 has been reported to exhibit strong ultraviolet reflectivity, suggesting potential applications in optical coatings and reflective materials.[13] Additional studies have demonstrated that optical behavior can vary substantially with chemical composition; for instance, differences have been observed between Ti_2AlC_2 and Cr_2AlC compounds.[14]

Substitution at the A-site also provides a pathway for tuning optical properties. Investigations of $Ti_3(Al_{1-x}Si_x)C_2$ have shown that gradual substitution of Al with Si can significantly modify optical anisotropy and reflectivity characteristics.[15,16] Similar trends have been reported for Cr_2AC phases, where variations in the A-element influence reflectivity and dielectric response.[17] These optical properties are closely related to the associated electronic structure and charge-carrier dynamics of the material. Consequently, analysing optical behaviour combined with structural and electronic properties provides critical insight into the electronic mechanisms governing conductivity and potential electrochemical performance in MAX phases.

In the present work, density functional theory calculations based on the projector augmented wave (PAW) method,[18] and appropriate exchange–correlation functionals[19] are employed to investigate the structural, electronic, and optical properties of Ti_3XC_2 (X = Ge, Pb, or Bi). Particular attention is given to the intercalation and deintercalation processes and their influence on lattice stability, electronic band structure, and optical response. The results provide new insights into the structural dynamics and electronic behavior of these MAX phases and highlight their potential relevance for advanced energy storage and electronic applications.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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