Electronic phase diagram established in Fe intercalated Weyl semimetal Td-MoTe2 for the first time

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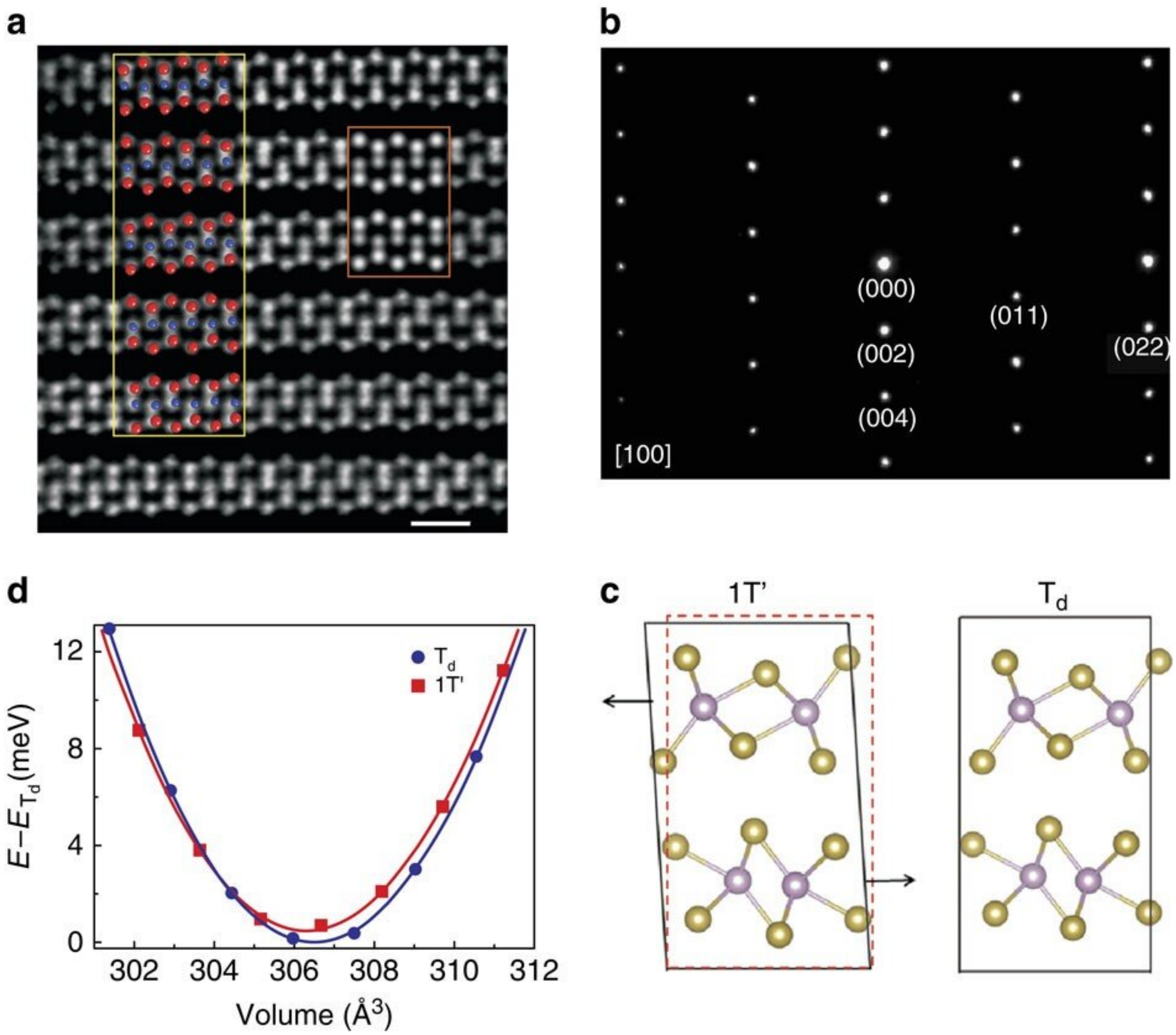

$MoTe_2$ crystal structure from another study. (a) HAADF-STEM image of

$1T'$-$MoTe_2$ along the [100] zone (scale bar, 0.5 nm). The red rectangle shows HAADF simulated image, and the red and blue spheres in the yellow rectangle represent Te and Mo atoms, respectively. (b) Corresponding electron diffraction images. (c) $1T'$ and T_d-$MoTe_2$ crystal structures. (d) Energy-volume dependence for $1T'$ and Td phases from DFT calculations. Credit: *Nature Communications* (2016). DOI: 10.1038/ncomms11038

In a study published in *Advanced Materials*, a research team led by Prof. Luo Xuan from Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences made a breakthrough in tuning electronic properties of Weyl semimetal T_d-$MoTe_2$ by intercalating 3d-element Fe atoms into the van der Waals (vdW) gap, which brought about exotic electronic behaviors as well as the first-time observed magnetic states in the topologically nontrivial Td phase.

The layered material Weyl semimetal T_d-$MoTe_2$ has attracted great attention due to its valuable properties including superconductivity, extreme large magnetoresistance, as well as topologically nontrivial band structure, making it an ideal hunting ground for exploring new physics and a promising candidate for fabricating new electronic devices.

Different ways have been used to controllably manipulate the electronic properties of T_d-$MoTe_2$, such as pressure, chemical substitution, low-dimensionality by mechanical exfoliation, but the research on the intercalation of transition-metal elements in Weyl semimetal T_d-$MoTe_2$ is still absent.

In this study, by improving the single crystal growth process, the 3d-element Fe intercalated T_d-Fe_xMoTe_2 samples were obtained. The team carried out systematic electrical, thermoelectric transport and ac susceptibility measurements, and studied the tunning effect of Fe intercalations in the system.

The team found that the 1T' to Td phase transition temperature (TS) of $MoTe_2$ gradually decreased with the increase of Fe intercalation, which was confirmed by different characterization results. Theoretical calculation suggested that the increased energy of Td phase, enhanced transition barrier and more occupied bands in 1T' phase were responsible for this phenomenon.

In addition, a $\rho^{\propto}$-ln T behavior induced by Kondo effect was observed with $x \geq 0.08$, due to the coupling between conduction carriers and the local magnetic moments of intercalated Fe atoms. A spin-glass transition occurred at about 10K in T_d-$MoTe_2$. The electronic phase diagram of T_d-$MoTe_2$ was established for the first time.

This study enriched the physical properties of Weyl semimetal T_d-$MoTe_2$ by 3d-element intercalation, and provided an ideal platform for in-depth understanding the correlation between the ground states and the interlayer coupling in layered transition metal dichalcogenides (TMDCs).

More information: Tianyang Wang et al, Origin of the Anomalous Electrical Transport Behavior in Fe-Intercalated Weyl Semimetal T d -MoTe 2, *Advanced Materials* (2023). DOI: 10.1002/adma.202208800

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