

surface can be readily obtained on creating a fresh surface. The origin of the SEA is attributed to the formation of sulfur vacancies in the surface of MoS_2 due to a slow desulfurization. This finding provides a new insight into the fundamental properties of TMD layer materials and is crucial for control of the conduction type and doping level of MoS_2 , and for 2D device development for ultrathin flexible transparent electronics. (Reported by Cheng-Maw Cheng)

This report features the work of Ruei-San Chen, Ya-

Ping Chiu, Cheng-Maw Cheng and their collaborators published in Nature Commun. 9, 1442 (2018)

TLS 21B1 U90 – (CGM) Angle-resolved UPS

- ARPES
- Materials Science, Condensed-matter Physics

Reference

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The Enigmatic Metal-Insulator Transition in Titanium Sesquioxide Ti_2O_3

The temperature dependent metal-insulator transition in titanium sesquioxide Ti_2O_3 has remained an unsolved problem for more than 60 years. Scientists have now succeeded to show that Ti_2O_3 exhibits strong correlation effects coupled with an increase in the structural distortion that drives the metal-insulator transition.

The temperature dependent metal-insulator transition (MIT) remains one of the most fascinating topics in materials science and condensed-matter physics. While the competition between Coulomb correlations and the energy bandwidth are the main source of localization and delocalization, it is often difficult to quantify and pinpoint their role in a MIT. The Mott-Hubbard transition is exemplified by V_2O_3 (V^{3+} ions $\equiv d^2$ electron system), which exhibits a temperature dependent first order MIT coupled to a structural distortion, and results in a low temperature antiferromagnetic insulator phase. In contrast, Ti_2O_3 , (Ti^{3+} ions $\equiv d^1$ electron system), which crystallizes in the same structure as V_2O_3 , exhibits a gradual MIT as a function of temperature without an accompanying structural or magnetic transition.^{1,2} Since titanium lies just next to vanadium in the periodic table, the physical properties of Ti_2O_3 has attracted significant attention since its discovery nearly 50 years ago. However, its electronic structure changes across the MIT had remained an enigmatic unsolved problem.

In a multinational collaboration spanning Europe and Asia, researchers have now succeeded to clarify and quantify the role of Coulomb correlations vis-à-vis changes in structural distortion without a crystal symmetry change in Ti_2O_3 . Early work emphasized the role of the so-called Ti-Ti c-axis dimer in Ti_2O_3 .³ However, band structure calculations without explicitly including on-site Coulomb correlations failed to pro-

duce an insulating ground state for Ti_2O_3 . In a careful study, L. Hao Tjeng (Max Planck Institute for Chemical Physics of Solids) and his co-workers have now revealed the direct role of strong Coulomb correlations

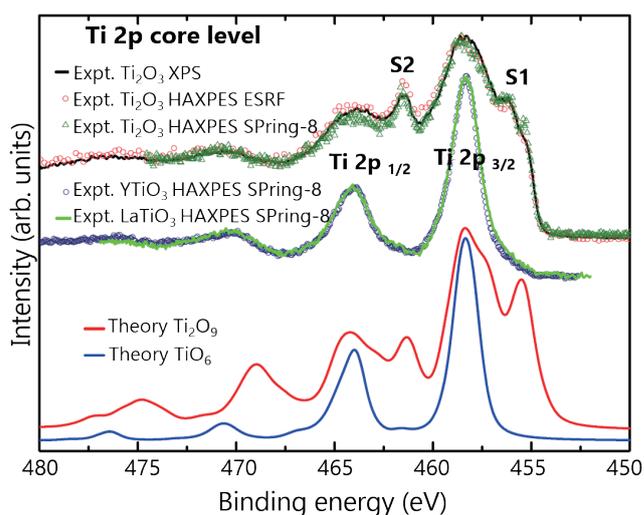


Fig. 1: Experimental Ti 2p core level photoemission spectra of Ti_2O_3 taken at 300 K with $h\nu = 1486.6$ eV (black line, XPS), $h\nu = 5931$ eV (red circle, HAXPES ESRF), and $h\nu \approx 6500$ eV (dark-green triangle symbol, HAXPES SPring-8), and experimental Ti 2p core-level photoemission spectra of YTiO_3 taken at 300 K (navy circle) and of LaTiO_3 taken at 200 K (green line) with $h\nu \approx 6500$ eV (HAXPES SPring-8). Also shown are the theoretical configuration-interaction calculations using the TiO_6 (blue line) and the Ti_2O_9 (red line) clusters. [Reproduced from Ref. 3]

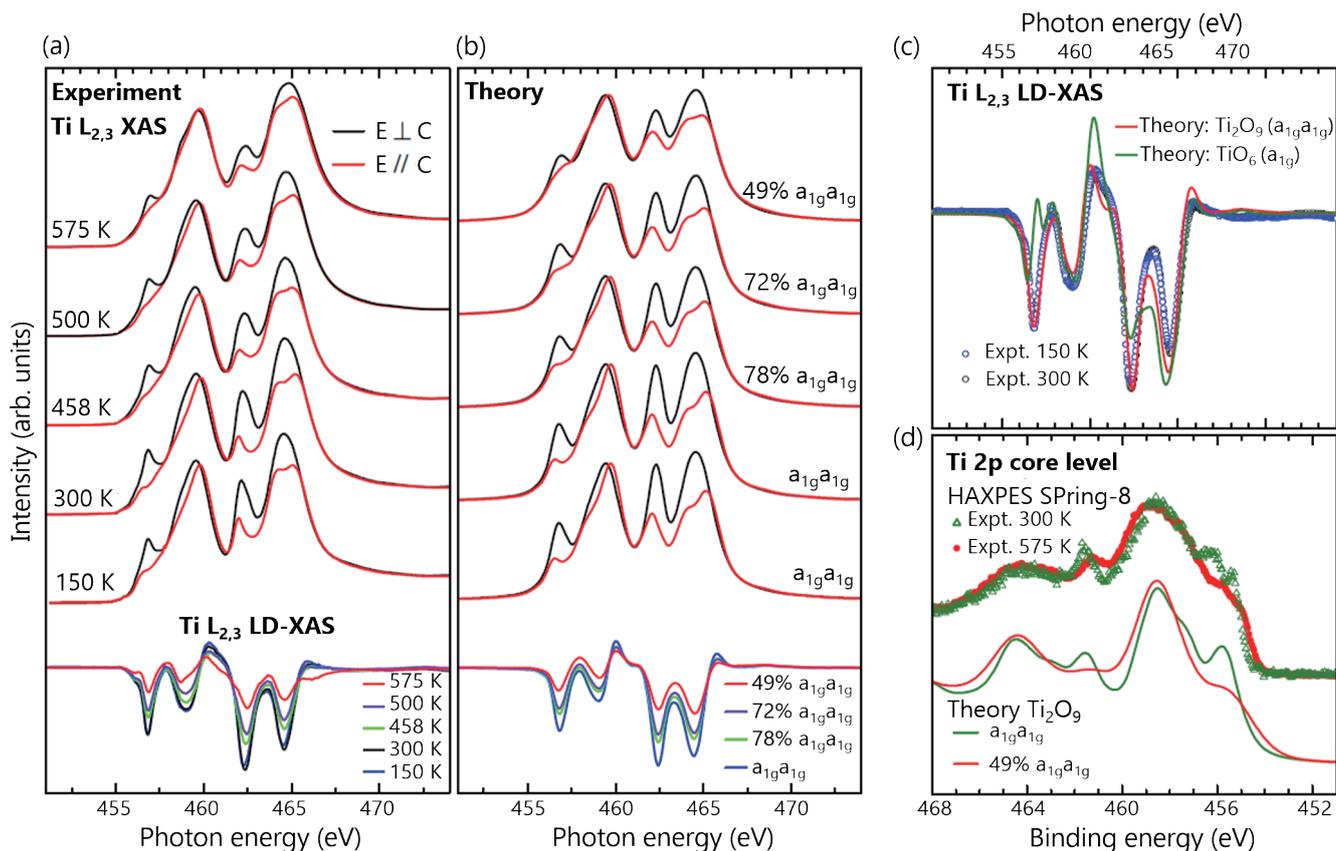


Fig. 2: (a) Experimental polarization dependent Ti L-edge XAS spectra of Ti_2O_3 measured at 150 K, 300 K, 458 K, 500 K and 575 K. (b) Calculated polarization-dependent $\text{Ti-L}_{2,3}$ XAS spectra for the corresponding temperatures using the Ti_2O_9 cluster. In the bottom of panels (a) and (b) are the corresponding linear dichroic (LD) spectra. (c) Close-up of the experimental LD spectrum in the low-temperature phase (blue and black circles) and the simulation using the TiO_6 (green line: a_{1g}) and the Ti_2O_9 (red line: $a_{1g}a_{1g}$) clusters. (d) Temperature dependence of the Ti 2p core-level spectrum and the simulations using the Ti_2O_9 cluster. [Reproduced from Ref. 3]

on the electronic structure of Ti_2O_3 . The authors showed that the bulk sensitive Ti 2p core level spectrum of the metal phase of Ti_2O_3 exhibits a very different line shape compared to the Ti 2p core level spectra of well-known Ti^{3+} oxides like YTiO_3 and LaTiO_3 (Fig. 1). Using configuration-interaction calculations, they showed that a single site TiO_6 model describes the spectra of YTiO_3 and LaTiO_3 well, but it cannot reproduce the experimental spectrum of Ti_2O_3 . However, calculations using an effective Hubbard model for a hydrogen molecule (which is equivalent to a Ti_2O_9 cluster) provides a reasonable explanation, not only for the Ti 2p core level spectrum, but also for the Ti 3d features in the valence band spectrum. This analysis allowed them to quantify the parameter $(U/t) \sim 3-4$, where U is the Coulomb energy and t is the hopping integral between the a_{1gA} and a_{1gB} orbitals on the two Ti sites A and B, respectively. This value of (U/t) confirms the importance of Coulomb correlations in the Ti-Ti dimer and indicates that the electronic parameters defining Ti_2O_3 are quite similar to V_2O_3 .

In addition, the authors also observed a strong linear dichroism in the Ti L-edge spectra from polarization dependent X-ray absorption spectroscopy (XAS) as a function of temperature (Fig. 2). Furthermore, they could also reproduce the experimentally observed linear dichroism using the Ti_2O_9 cluster calculations. In particular, the results showed that the temperature dependence of the Ti L-edge linear dichroism is due to systematic changes in the orbital occupancies. They could also show that the temperature dependence of the Ti 2p core level photoemission spectra could be reproduced with the same calculations. Finally, the authors carried out temperature dependent valence band photoemission and O K-edge XAS. The spectra showed a clear gap formation in the occupied valence band and unoccupied conduction band states due to gradual changes as a function of temperature across the MIT (Fig. 3). The authors concluded their study by saying that their results validate the original model of Goodenough² with the added role of strong effective Coulomb correlations in Ti_2O_3 . (Reported by Ashish Chainani)

This report features the work of L. Hao Tjeng and his co-workers published in *Phys. Rev. X* **8**, 021004 (2018).

TLS 11A1 BM – (Dragon) MCD, XAS SP 12U2 HAXPES/Photoemission

- XANES, X-ray Linear Dichroism, Hard X-ray Photoemission Spectroscopy
- Metal-insulator Transitions, Strongly Correlated Electron Systems

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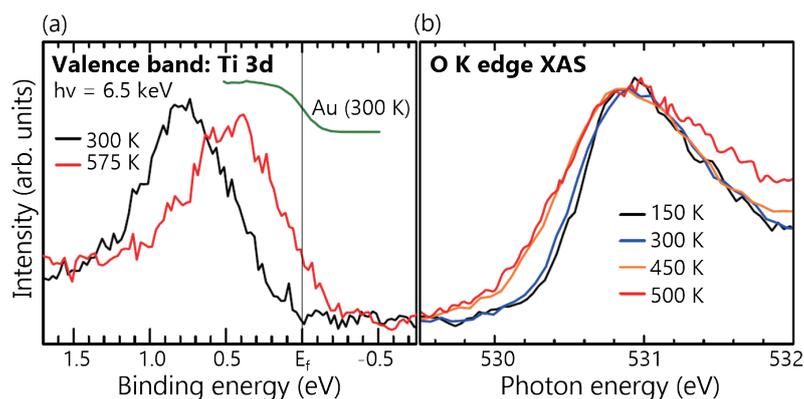


Fig. 3: (a) Close-up of the temperature dependence of the valence-band spectra of Ti_2O_3 taken with $h\nu \approx 6.5$ keV (HAXPES SPring-8), together with the Au Fermi cutoff as E_F reference. (b) Close-up of the temperature dependence of the O K-edge XAS spectra of Ti_2O_3 . [Reproduced from Ref. 3]

Dynamic Ferrimagnetism in a Double Perovskite

Researchers have succeeded to synthesize a new double perovskite oxide Y_2CoRuO_6 which shows dynamic ferrimagnetism in the form of spin-glass properties at temperatures below the long range ferrimagnetic ordering temperature.

Double perovskite oxides have the general chemical formula $\text{A}_2\text{BB}'\text{O}_6$, where the A-site ion often forms a closed shell ionic configuration, while B and B' are 3d/4d/5d transition metal ions which can take up a general magnetically active d^n configuration.¹ Due to the very large combination of B and B'-site transition metal cations which can form the double perovskite structure, it has tremendous potential to show a variety of magnetic and electrical properties. Although the A-site ions may not be magnetically active themselves, it is well-known that the size of the A-site ion provides a structural control of the magnetic superexchange interaction of the B, B'-site ions.¹ In this highlight, we discuss one such successful case of controlled synthesis and magnetic properties of the series $\text{La}_{2-x}\text{Y}_x\text{CoRuO}_6$. The A-site substitution of La with Y content x , from $x = 0$ to 1, allows a tuning of the magnetic ground states from an antiferromagnetic insulator to spin-glass to a ferrimagnetic insulator. The authors used several techniques including diffraction, spectroscopy, DC magnetization, time dependent isothermal magnetization and frequency dependent ac-susceptibility measurements to obtain conclusive evidence of dynamic ferrimagnetism in Y_2CoRuO_6 .²

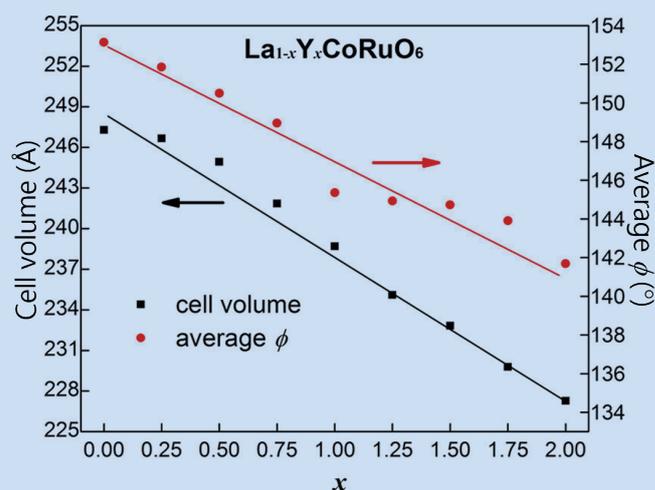


Fig. 1: Crystal structure analyses of $\text{La}_{2-x}\text{Y}_x\text{CoRuO}_6$ ($x = 0-1.0$) samples showing a systematic evolution of the unit cell volume and the B-O-B' angle ϕ . [Reproduced from Ref. 2]

In a multinational collaboration carried out by Martha Greenblatt (Rutgers University) and her co-workers, polycrystalline $\text{La}_{2-x}\text{Y}_x\text{CoRuO}_6$ ($x = 0-1.0$) samples were synthesized using the conventional solid state reaction method and characterized for their crystal