Magneto-lattice coupling in charge modulated intercalated transition metal dichalcogenides

Arunava Kar[1,*]
Artem Korshunov[1], David Subires[1], Chan-young Lim[1], Alex Frano[2], Victor Pardo[3] and Santiago Blanco-Canosa[1,4]
[1]*Donostia International Physics Center (DIPC), San Sebastian, Spain.*
[2]*Department of Physics, University of California San Diego, San Diego, California 92093, USA.*
[3]*Departamento de Fısica Aplicada, Universidade de Santiago de Compostela, E-15782 Campus Sur s/n, Santiago de Compostela, Spain.*
[4]*KERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain.*
*phys.arunava20@gmail.com

The large van der Waals gap in transition metal dichalcogenides (TMDs) offers a playground to host external metal atoms that modify the ground state of these 2D materials. Here, we experimentally and theoretically address a new charge density wave (CDW) phase in a family of intercalated TMDs. While short-range charge fluctuations develop in $Co_{1/3}TaS_2$ and $Fe_{1/3}TaS_2$, the long-range CDW switches-on in $Fe_{1/3}NbS_2$ are driven by the interplay of magnetic order and lattice degrees of freedom. The magnetoelastic coupling is demonstrated in $Fe_{1/3}NbS_2$ by enhancing the charge modulations upon the magnetic field below T_N, although Density functional perturbation theory (DFPT) calculations predict negligible electron(spin)-phonon coupling. Furthermore, we show that Co-intercalated TaS_2 displays a Kagome-like Fermi surface, hence opening the path to engineer electronic band structures and study the entanglement of spin, charge, and spin-phonon mechanisms in the large family of intercalated TMDs.

References

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Figure:

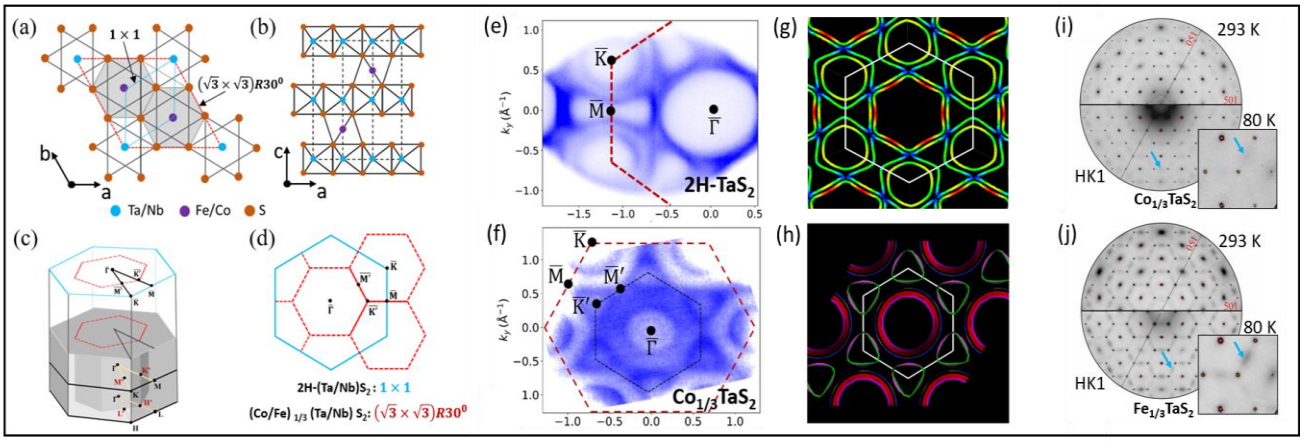

Figure 1: (a)-(b) Geometric structure of $(Fe/Co)_{1/3}(Ta/Nb)S_2$, viewed along c and b axis, respectively. (c)-(d) Bulk and surface projected First Brillouin zone of 1/3 Transition metal intercalated 2Ha-TMDC systems. The side of superstructure BZ is shrined by $(1/\sqrt{3})$ amount of the 1x1 BZ of the parent compounds and also rotated by 30^0. (e)-(f) Experimental FS of 2H-TaS_2 and $(Co)_{1/3}TaS_2$ obtained in ARPES, while (g)-(h) are DFT computed FS in the corresponding materials. (i)-(j) Diffuses scatted spectra obtained in HK1 plane in $Co_{1/3}TaS_2$ and $Fe_{1/3}TaS_2$, respectively.