On-Site Coulomb Energy in TMDC Compounds by Resonant Photoemission

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Abstract. The Coulomb interaction U serves as a pivotal parameter influencing electron behavior, particularly accentuated within low-dimensional materials. Transition Metal Dichalcogenides, quasi-2-D systems, exhibit diverse electronic traits like CDW order, co-existing CDW with superconductivity, and topologically non-trivial phases. Their 2D nature intensifies coulomb interaction of electrons, leading to phenomena like Mott-Hubbard transitions.

The on-site Coulomb energy for transition metal and chalcogenide atoms is determined through a method proposed by Cini and Sawatzky [1-3]. This approach is based on comparison of the energy of the correlation satellite linked to the two-valence-hole (VV)Auger final state in resonant photoemission with the uncorrelated two-valence-hole energies derived from a self-convolution of single-hole states obtained from a non-resonant photoemission spectrum. The energy difference between the main peaks of the resonantly enhanced spectrum and the uncorrelated two-hole spectrum serves as a measure of the Coulomb energy.

Here we aim to determine the on-site Coulomb interaction for each element within two series of TMDC materials (MX_2, where X = S, Se, Te and M = Nb, Ta) by resonant ARPES.

REFERENCES

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