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Magnetic Moment Collapse-Driven Mott Transition in MnO¹

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Metal-insulator transition in strongly correlated electron systems has been one of the central themes of condensed matter physics for a few decades. In the simplest model system, the single band Hubbard model, the transition, which is still not completely understood, is driven by the ratio of the on-site repulsion to the bare bandwidth. Real materials with multiple bands offer possibility of alternative scenarios of the metal-insulator transition. In this talk we will present a numerical study of MnO under high pressure using combination of the standard bandstructure theory and modern many-body methods (dynamical mean-field theory). Our results reveal a close relationship between the high-spin to low-spin transition and metallization, which can be interpreted as the moment collapse driving the metallization. We find an isostructural volume collapse of about 13% accompanying the transition. While the moment collapse, which is essentially an atomic effect, is obtained by most electronic structure methods, the metal-insulator transition can be described reliably only when dynamical correlations are taken into account. We find our results to compare very well to the available experimental data. In order to demonstrate the capability of the computational method PES and ARPES spectra obtained on the related NiO with and without hole doping will also be presented.

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