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【605】 Interplay between the structural and metal-insulator transition in rare-earth nickelates

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Rare-earth nickelates, RNiO_3 , represent an intriguing example of materials with a highly tunable metal-insulator transition (MIT) and high potential for heterostructure engineering. The T -dependent paramagnetic MIT observed both in the bulk and ultrathin films of RNiO_3 is almost always accompanied by a subtle crystal-structure transformation, resulting in disproportionation of Ni-O bonds. We employ recent advances in understanding the nature of the insulating phase in RNiO_3 to unravel the mechanism underlying the combined structural/metal-insulator transition. By explicitly including lattice degrees of freedom into the description we show how a peculiar electronic structure may result in stabilization of the bond-disproportionated phase and we identify two control parameters associated with the transition.

Author: PEIL, Oleg (Université de Genève)

Presenter: PEIL, Oleg (Université de Genève)

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