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Metastable low-spin character of Co^{2+} and the control of spin state transition BONGJAE KIM, B. I. MIN, POSTECH — We have studied different spin states of the octahedrally coordinated Co^{2+} systems. For every tested systems, we found metastable character of low-spin phase and, interestingly, the energy differences between the high-spin and low-spin phases are similar regardless of the anion (X) type, Co^{+2}-X bond lengths and CoX_6 octahedron distortion. For $CoCl_2$ as a model system, we studied pressure-induced high-spin to low-spin state transition, which is governed by J/Δ_{CF} value (J: exchange parameter, Δ_{CF}: crystal-field parameter). $CoCl_2$ shows sudden collapse of volume and spin moment at the point of spin state transition together with the insulator-to-metal transition. Unlike the other transition-metal oxides, which shows pressure-driven Mott-type transition, physics of $CoCl_2$ is determined mainly by J and Δ_{CF}, not by U and W.

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