**First-principles-based calculation of branching ratio for 5*d*, 4*d*, and 3*d* transition metal systems**

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A first-principles computation scheme to calculate ‘branching ratio’ in x-ray absorption spectroscopy has been applied to various 5*d*, 4*d*, and 3*d* transition-metal elements and compounds. This new method is based on an atomic theory which assumes the atomic core hole interacts barely with valence electrons [1, 2]. While it provides an efficient way to calculate the experimentally measurable quantity without generating spectrum itself, its reliability and applicability should be carefully examined especially for the light transition metal systems. Here we select 30 different materials and compare the calculation results with experimental data. It is found that our scheme well describes 5*d* and 4*d* transition metal systems whereas, for 3*d* materials, the difference between the calculation and experiment is observed. The difference for 3*d* transition metal system is attributed to the neglect of core-valence interaction. We expect that our results shed light on the applicability of the method.

1. J.-H. Sim, H. Yoon, S. H. Park, and M. J. Han, Physical Review B 94, 115149 (2016)
2. B. T. Thole and G. van der Laan, Physical Review A 38, 1943 (1988)