Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2018

L-edge sum rule analysis on 3d transition metal sites: from d^{10} to d^0 and towards application to extremely dilute metallo-enzymes

Hongxin Wang,[1,2,*], Stephan Friedrich[3], Lei Li[4], Ziliang Mao[1], Pinghua Ge[5], Mahalingam Balasubramanian[6], and Daulat S. Patil[2]

[1] Department of Chemistry, University of California, Davis, CA 95616, USA
[2] Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
[3]Lawrence Livermore National Laboratory, Advanced Detectors Group, 7000 East Avenue, Livermore, CA 94550, USA
[4] Synchrotron Radiation Nanotechnology Center, University of Hyogo, 1-490-2 Kouto, Shingu-cho, Tatsuno, Hyogo 679-5165, Japan
[5] Department of Physics, University of Illinois, 1110 West Green St., Urbana, IL 61801, USA
[6] Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, USA

Supplemental Information

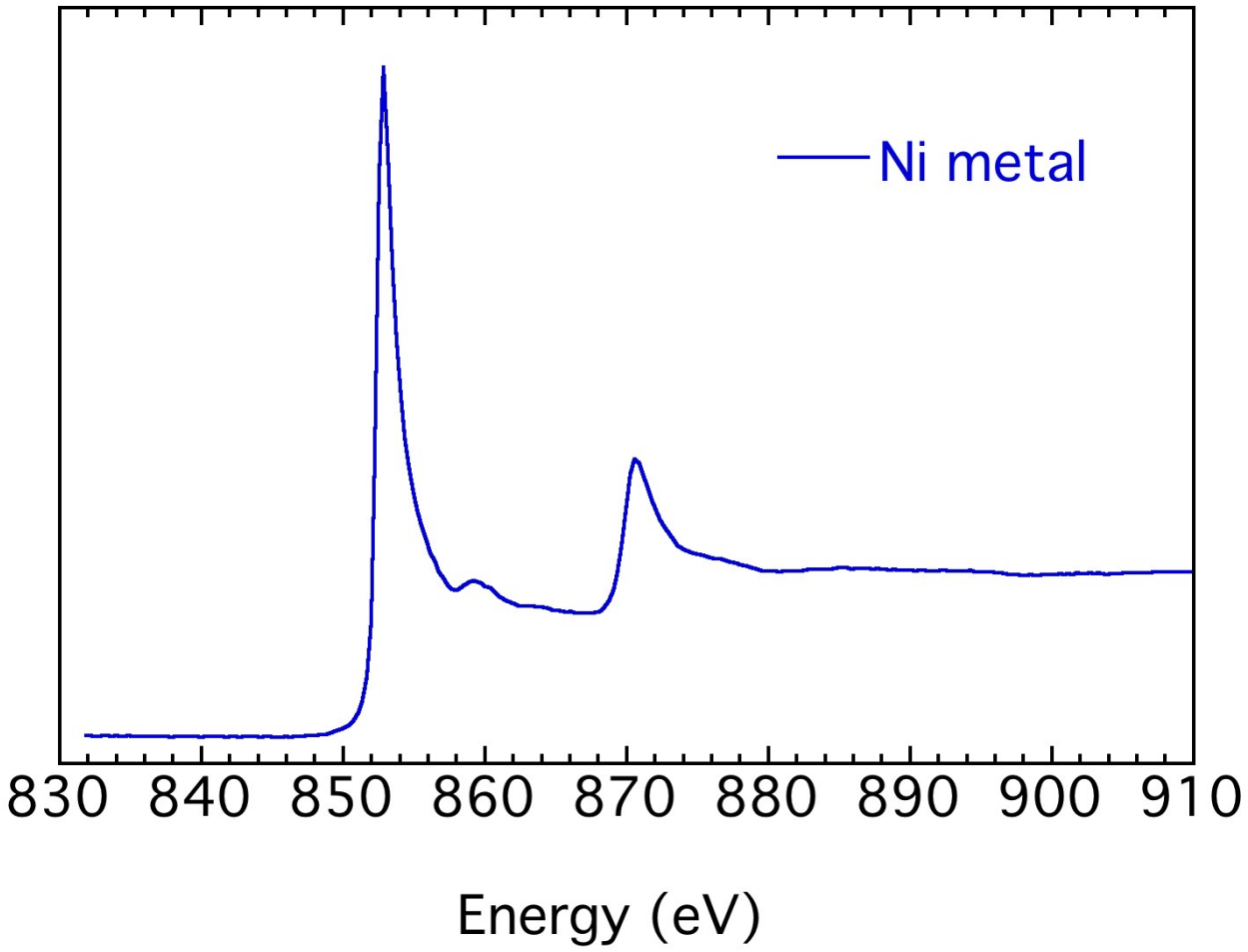

Figure S1 The Ni L XAS for Ni metal. The L XAS feature is similar with a $3d^8$ compound, such as NiF2.

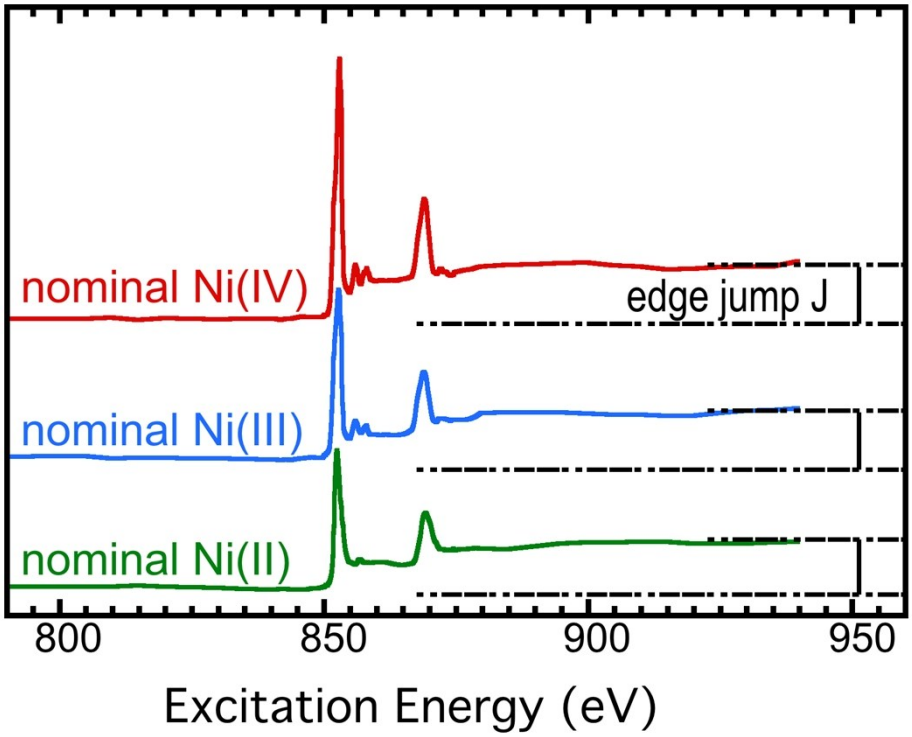

Figure S2 The Ni L XAS for ultra-covalent $(Ph_4As)_2Ni[S_2C2(CF_3)_2]_2$ (50.5%), $(^nBu_4N)Ni[S_2C_2(CF_3)_2]_2$ (44.0%) and $Ni[S_2C_2(CF_3)_2]_2$ (38.5%) complexes.

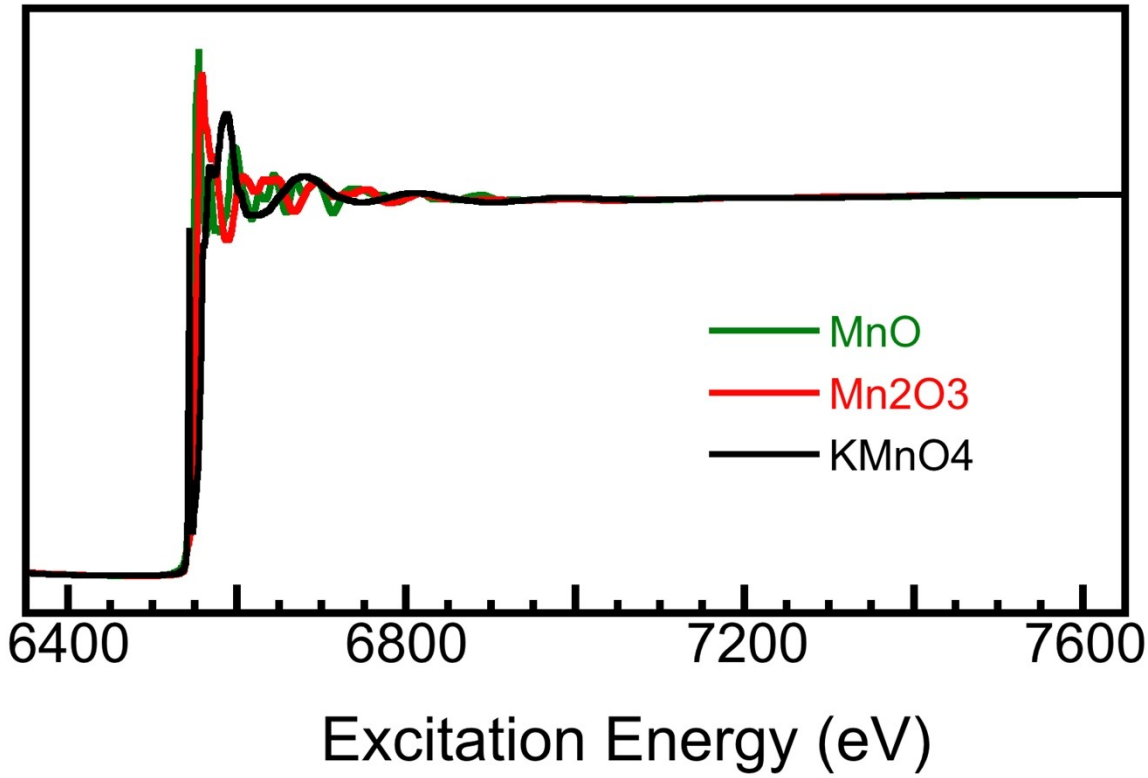

Figure S3 The Mn K XAS for MnO (green), Mn_2O_3 (red) and $KMnO_4$ (black), including their EXAFS regions.