Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Giant Negative Magnetoresitance in Ni(quinoline-8-selenoate)$_2$

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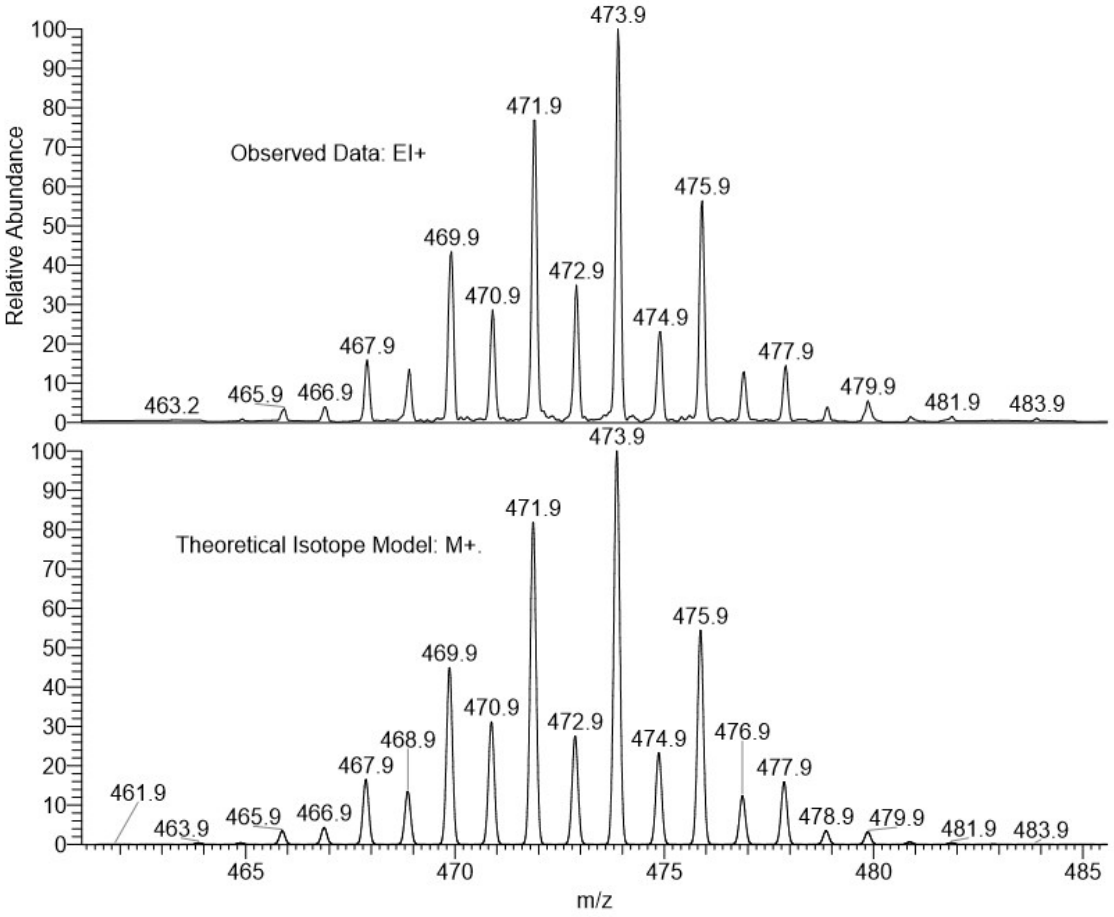

Figure S1: Mass spectrum of [Ni(qs)$_2$]; acquired spectrum (top), theoretical isotope pattern (bottom).

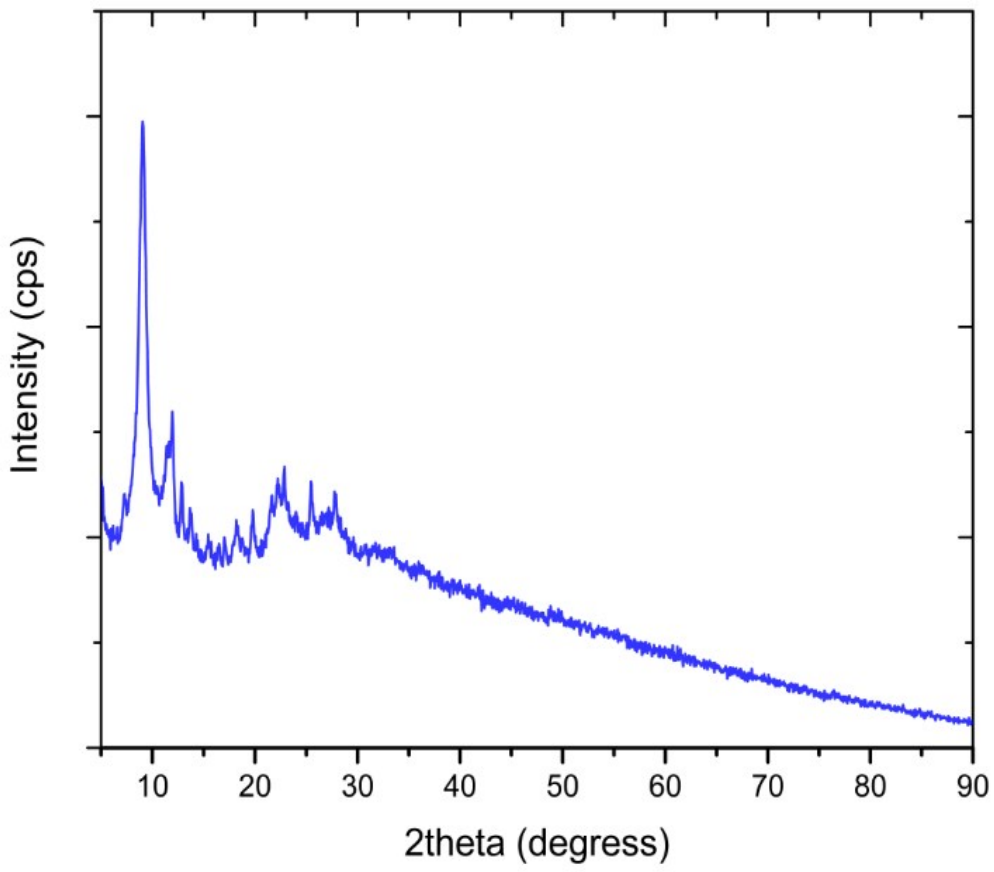

Figure S2: PXRD obtained for [Ni(qs)$_2$].

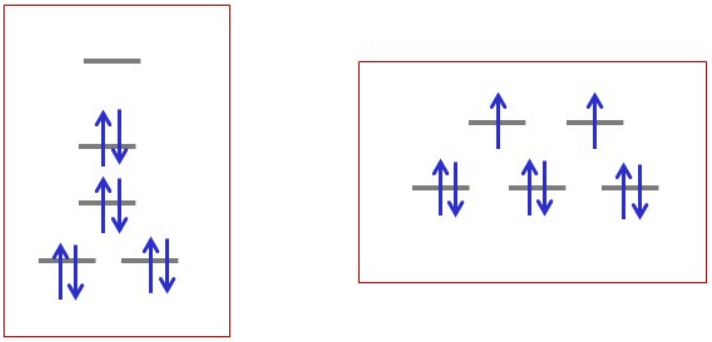

Figure S3: Illustration of crystal-field splitting and d-orbital occupancy for d^8 Ni(II) in ideal square-planar (left) and octahedral (right) geometry, showing diamagnetic and paramagnetic character respectively.

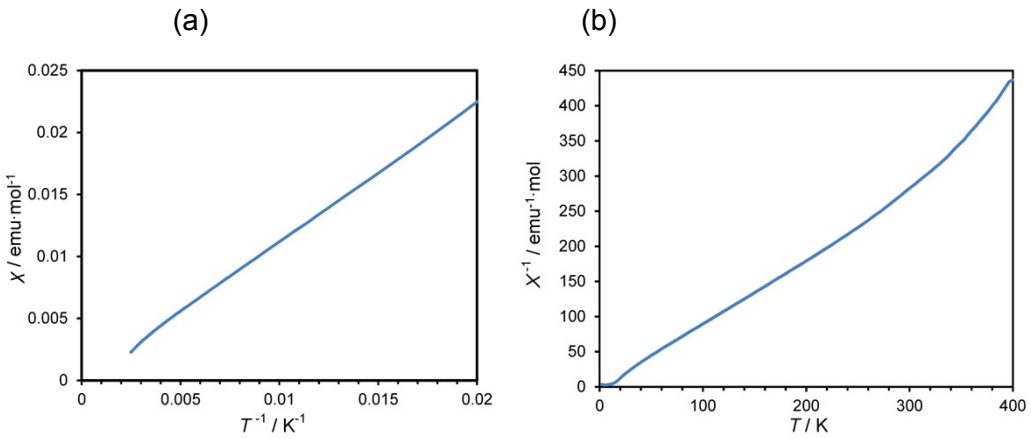

Figure S4: χ-T^{-1} (a) and χ^{-1}-T plot (b) of the magnetic susceptibility of $Ni(qs)_2$. Temperature-independent component (the contribution of diamagnetic component and ferromagnetic impurity) was evaluated and subtracted by setting the intersection of the linear region of χ-T^{-1} to 0 (high-temperature approximation).

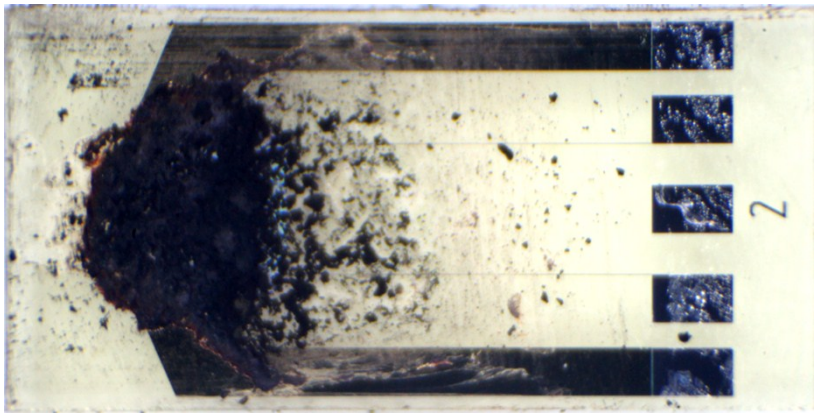

Figure S5: Powdered sample of $[Ni(qs)_2]$ on an interdigitated circuit used for conductivity and magnetoresistance measurements.

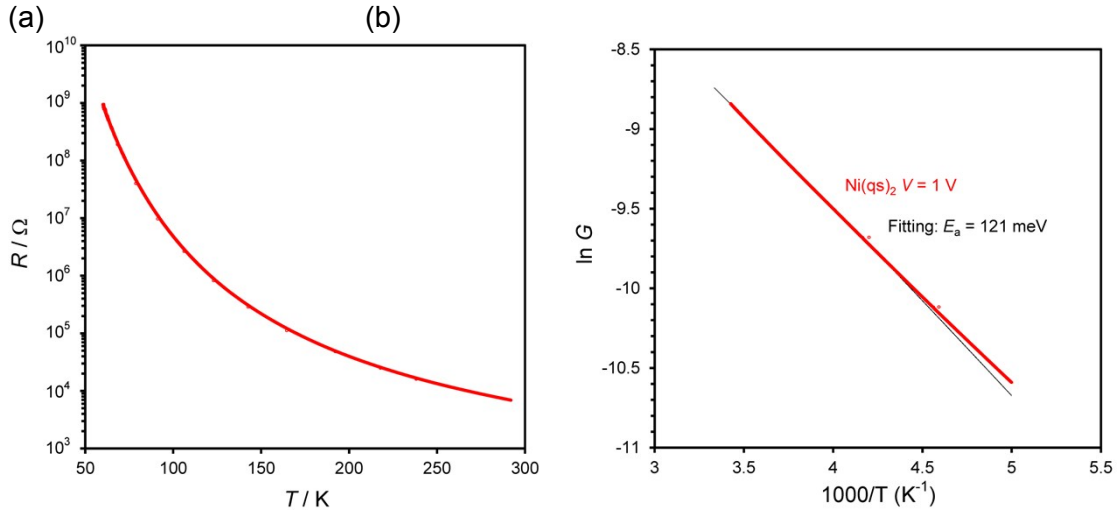

Figure S6: Temperature dependence of the resistance of $Ni(qs)_2$ micro-crystals deposited on a inter-digitated micro-gap electrodes (a) and the Arrhenius plot from the obtained result (b). Measurements were carried through the current-measurement with a constant applied-voltage (1V) condition. Activation energy E_a = 121 meV was estimated from the Arrhenius plot between

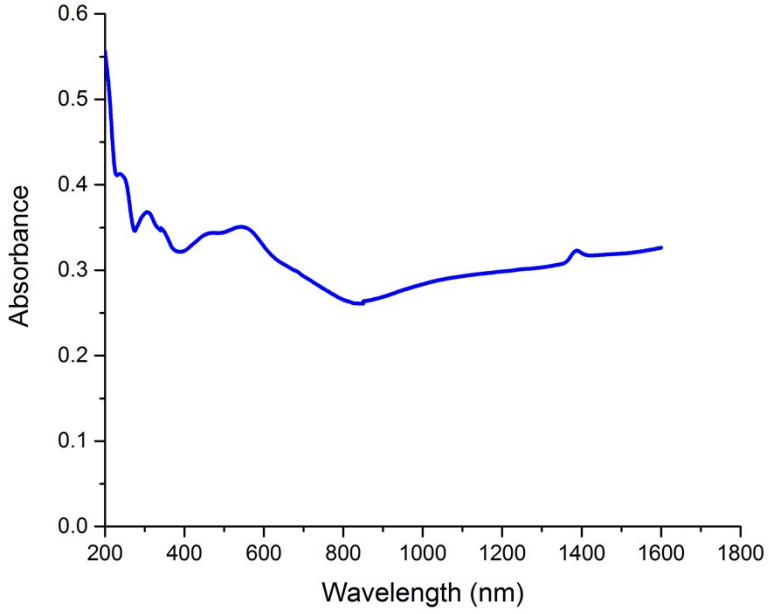

Figure S7: Absorbance of $[Ni(qs)_2]$ determined by diffuse reflectance spectroscopy.

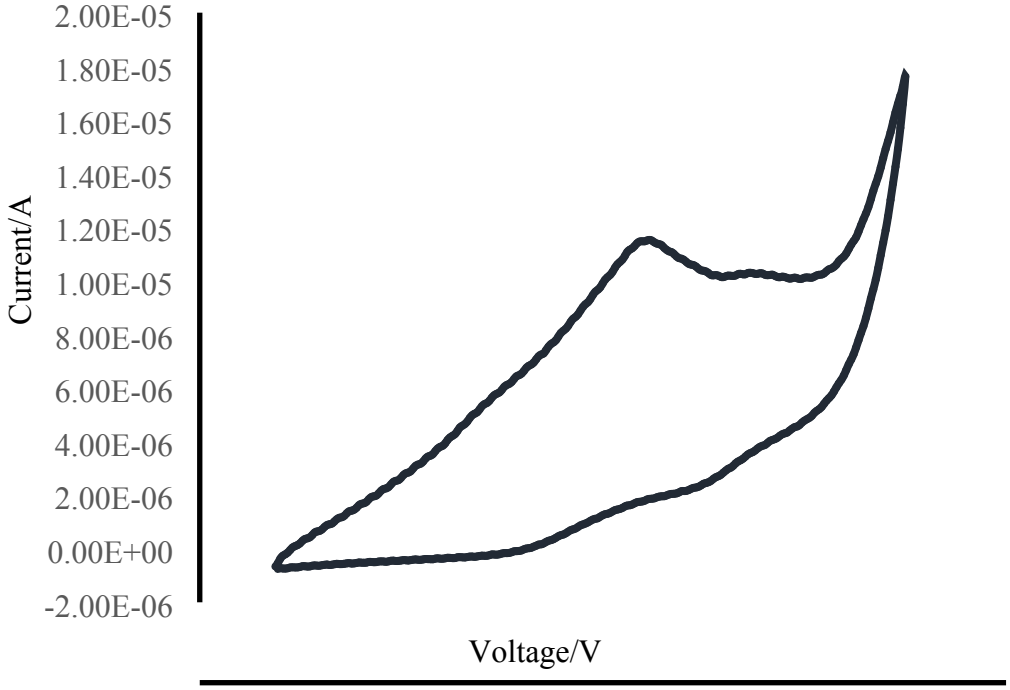

Figure S8: Cyclic voltammogram of solid $[Ni(qs)_2]$. Measured in 0.1 M solution of $[TBA][PF_6]$ in acetonitrile. Sample material was pseudo-dropcast onto 3mm Pt working electrode surface and allowed to dry before measurement was made.

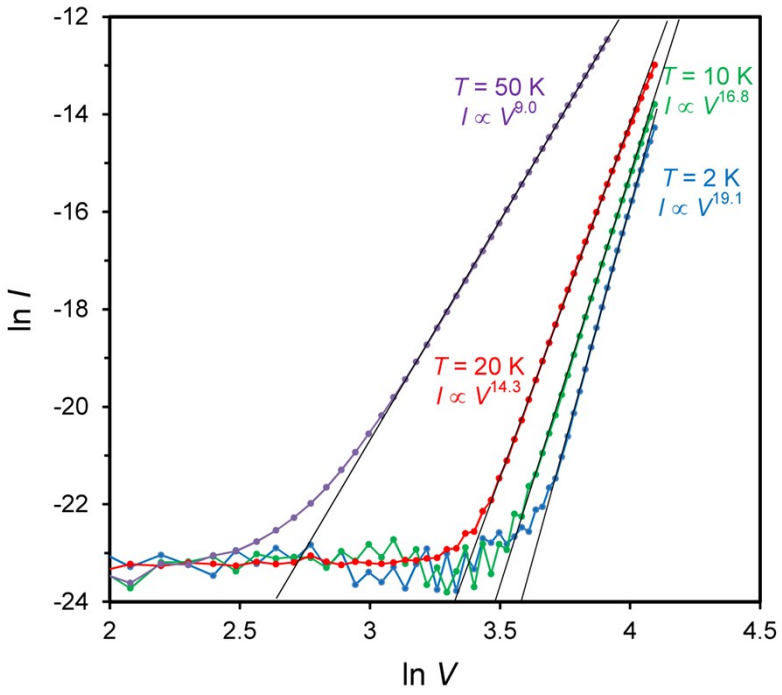

Figure S9: Log-log plot of the *I-V* characteristics (Figure 3) of $Ni(qs)_2$ in the lower temperatures. The linear relation in the log-log plot means the higher-order *I-V* characteristics.

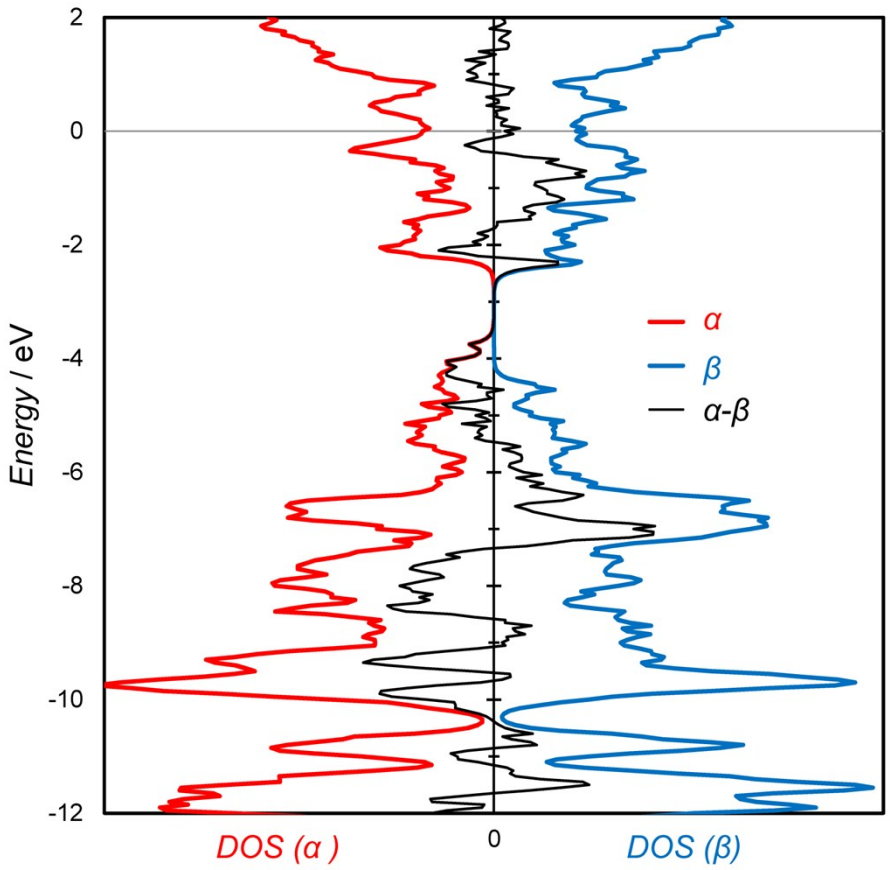

Figure S10: Density of states (DOSs) of the $Ni(qs)_2$ 8mer, obtained from the calculation result for Figures 5 and 6 (UB3LYP/TZVP). Occupied band edges (just below the Fermi energy, *ca.* 3eV) have big energy difference (>0.5eV) between α and β spins. Spin-polarized transport is expected from this band structure. This big spin-polarization is caused by the local spin on Ni(II) ions.