Supporting Information for:
Synergy of Binary Substitutions for Improving the Cycle Performance in LiNiO$_2$ Revealed by Ab Initio Materials Informatics

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Table S 1: $\Delta d_{\text{ave}}$ for unary substitution.

| Element | $\Delta d_{\text{ave}}$ (Å) | Element | $\Delta d_{\text{ave}}$ (Å) | Element | $\Delta d_{\text{ave}}$ (Å) |
|---------|-----------------|---------|-----------------|---------|-----------------|
| V       | 0.124           | Pt      | 0.147           | Ag      | 0.199           |
| Nb      | 0.125           | Ho      | 0.148           | Gd      | 0.216           |
| Ge      | 0.132           | In      | 0.149           | Ce      | 0.257           |
| Ir      | 0.134           | Er      | 0.149           | Eu      | 0.283           |
| Au      | 0.134           | Sc      | 0.150           | Tl      | 0.290           |
| Al      | 0.135           | Sn      | 0.155           | Pm      | 0.306           |
| Ti      | 0.135           | Pb      | 0.159           | Sm      | 0.314           |
| Ta      | 0.135           | Pa      | 0.160           | Hg      | 0.337           |
| Mg      | 0.135           | Hf      | 0.160           | Na      | 0.347           |
| Ga      | 0.137           | Rh      | 0.161           | Th      | 0.385           |
| Ru      | 0.137           | Fe      | 0.161           | Nd      | 0.395           |
| Bi      | 0.139           | Cu      | 0.162           | Pr      | 0.420           |
| Dy      | 0.139           | Po      | 0.163           | Sr      | 0.426           |
| Os      | 0.140           | W       | 0.165           | La      | 0.440           |
| Sb      | 0.140           | Zn      | 0.167           | Ac      | 0.493           |
| Mn      | 0.141           | Cr      | 0.167           | Ba      | 0.574           |
| Tc      | 0.141           | Zr      | 0.169           | Ra      | 0.622           |
| Y       | 0.142           | Pd      | 0.172           | K       | 0.685           |
| Tb      | 0.143           | Mo      | 0.177           | Rb      | 0.777           |
| Re      | 0.144           | Ca      | 0.189           | Fr      | 0.856           |
| Tm      | 0.146           | Yb      | 0.191           | Cs      | 0.865           |
| Lu      | 0.147           | Cd      | 0.193           |         |                 |
Table S 2: $\Delta d_{\text{ave}}$ for binary substitution.

| Elements | $\Delta d_{\text{ave}}$ (Å) | Elements | $\Delta d_{\text{ave}}$ (Å) | Elements | $\Delta d_{\text{ave}}$ (Å) |
|----------|-----------------------------|----------|-----------------------------|----------|-----------------------------|
| GeSn     | 0.386                       | SrTa     | 0.448                       | AlGa     | 0.139                       |
| VTh      | 0.431                       | VIr      | 0.127                       | MnPt     | 0.131                       |
| ZnRu     | 0.166                       | ZrPt     | 0.194                       | FeGa     | 0.125                       |
| FePt     | 0.168                       | MnMo     | 0.166                       | CrRu     | 0.129                       |
| EuPt     | 0.473                       | CuBi     | 0.150                       | CrOs     | 0.133                       |
| CuNb     | 0.145                       | DyPt     | 0.461                       | CrFe     | 0.133                       |
| VGa      | 0.114                       | NbGd     | 0.653                       | TiRh     | 0.160                       |
| ErLu     | 0.484                       | ErOs     | 0.433                       | FeNb     | 0.158                       |
| VFe      | 0.136                       | CdTa     | 0.554                       | MnZn     | 0.160                       |
| SnEr     | 0.240                       | SnYb     | 0.144                       | AlTl     | 0.247                       |
| FeNd     | 0.489                       | CrLu     | 0.132                       | CuYb     | 0.176                       |
| HoOs     | 0.431                       | TiFe     | 0.116                       | MgCr     | 0.109                       |
| SnPr     | 0.359                       | CrZn     | 0.146                       | CrGe     | 0.136                       |
| IrRa     | 0.693                       | VMn      | 0.129                       | FeIr     | 0.135                       |
| CrHg     | 0.128                       | AlFe     | 0.130                       | CrPt     | 0.139                       |
| SrZr     | 0.469                       | AlMn     | 0.123                       | CrRe     | 0.083                       |
| ZnHg     | 0.373                       | NaPt     | 0.314                       | GeHf     | 0.291                       |
| CdSn     | 0.474                       | GaHo     | 0.256                       | GeCd     | 0.231                       |
| SnSb     | 0.391                       | VTa      | 0.127                       | GaNb     | 0.278                       |
| AgHf     | 0.164                       | NbHf     | 0.336                       | ZnOs     | 0.145                       |
| PdAu     | 0.186                       | AlHf     | 0.215                       | MnRe     | 0.146                       |
| ReTl     | 0.475                       | AlCr     | 0.123                       | CuRe     | 0.153                       |
| PdCe     | 0.470                       | MgPt     | 0.133                       |
| OsHg     | 0.368                       | MgCu     | 0.124                       |