Supplementary material to:

K.T. Malatji, D. Santos-Carballal, U. Terranova, P.E. Ngoepe and N.H. de Leeuw,

Controlling the Lithium Intercalation Voltage in the $Li(Mn_{1-x}Ni_x)_2O_4$ Spinel *via* Tuning of the Ni Concentration: a Density Functional Theory Study,

S. Afr. J. Chem., 2021, **74** (Special Edition), 3–7.

Supplementary information, *S. Afr. J. Chem.*

Controlling the lithium intercalation voltage in the $Li(Mn_{1-x}Ni_x)_2O_4$ spinel via tuning of the Ni concentration: a Density Functional Theory study

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1. Optimised lattice geometry and ionic positions for $LiMn_2O_4$

Format: VASP POSCAR file

```
Li Mn O
   1.0000000000000000
     8.3395017889305052    0.0000000000000000   -0.0000000000000000
     0.0000000000000000    8.3395017889305052   -0.0000000000000000
    -0.0000000000000000    0.0000000000000000    8.3395017889305052
   Li   Mn   O
     8    16    32
Direct
  0.1250000000000000  0.1250000000000000  0.1250000000000000
  0.6250000000000000  0.1250000000000000  0.6250000000000000
  0.1250000000000000  0.6250000000000000  0.6250000000000000
  0.6250000000000000  0.6250000000000000  0.1250000000000000
  0.8750000000000000  0.3750000000000000  0.3750000000000000
  0.8750000000000000  0.8750000000000000  0.8750000000000000
  0.3750000000000000  0.3750000000000000  0.8750000000000000
  0.3750000000000000  0.8750000000000000  0.3750000000000000
  0.5000000000000000  0.5000000000000000  0.5000000000000000
  0.2500000000000000  0.7500000000000000  0.0000000000000000
  0.7500000000000000  0.0000000000000000  0.2500000000000000
  0.0000000000000000  0.2500000000000000  0.7500000000000000
  0.7500000000000000  0.2500000000000000  0.0000000000000000
  0.2500000000000000  0.0000000000000000  0.7500000000000000
  0.0000000000000000  0.7500000000000000  0.2500000000000000
  0.5000000000000000  0.0000000000000000  0.0000000000000000
  0.2500000000000000  0.2500000000000000  0.5000000000000000
  0.7500000000000000  0.5000000000000000  0.7500000000000000
  0.7500000000000000  0.7500000000000000  0.5000000000000000
  0.2500000000000000  0.5000000000000000  0.2500000000000000
  0.0000000000000000  0.5000000000000000  0.0000000000000000
  0.5000000000000000  0.2500000000000000  0.2500000000000000
  0.5000000000000000  0.7500000000000000  0.7500000000000000
  0.0000000000000000  0.0000000000000000  0.5000000000000000
  0.2621894965390581  0.2621894965390581  0.2621894965390581
  0.4878105034609419  0.9878105034609419  0.7621894965390581
  0.9878105034609419  0.7621894965390581  0.4878105034609419
  0.7621894965390581  0.4878105034609419  0.9878105034609419
  0.0121894965390581  0.5121894965390581  0.2378105034609419
  0.7378105034609419  0.7378105034609419  0.7378105034609419
  0.5121894965390581  0.2378105034609419  0.0121894965390581
  0.2378105034609419  0.0121894965390581  0.5121894965390581
  0.5121894965390581  0.0121894965390581  0.2378105034609419
  0.0121894965390581  0.2378105034609419  0.5121894965390581
  0.2378105034609419  0.5121894965390581  0.0121894965390581
  0.9878105034609419  0.4878105034609419  0.7621894965390581
  0.4878105034609419  0.7621894965390581  0.9878105034609419
  0.7621894965390581  0.9878105034609419  0.4878105034609419
  0.2621894965390581  0.7621894965390581  0.7621894965390581
  0.4878105034609419  0.4878105034609419  0.2621894965390581
  0.9878105034609419  0.2621894965390581  0.9878105034609419
  0.0121894965390581  0.0121894965390581  0.7378105034609419
  0.7378105034609419  0.2378105034609419  0.2378105034609419
  0.5121894965390581  0.7378105034609419  0.5121894965390581
  0.5121894965390581  0.5121894965390581  0.7378105034609419
  0.0121894965390581  0.7378105034609419  0.0121894965390581
  0.9878105034609419  0.9878105034609419  0.2621894965390581
  0.4878105034609419  0.2621894965390581  0.4878105034609419
  0.7621894965390581  0.2621894965390581  0.7621894965390581
  0.2621894965390581  0.4878105034609419  0.4878105034609419
  0.2378105034609419  0.7378105034609419  0.2378105034609419
```

2. Optimised lattice geometry and ionic positions for $LiNi_2O_4$

Format: VASP POSCAR file

```
Li Ni O
   1.0000000000000000
     8.0317498321027472    0.0000000000000000    0.0000000000000000
    -0.0000000000000000    8.0317498321027472    0.0000000000000000
    -0.0000000000000000   -0.0000000000000000    8.0317498321027472
   Li   Ni   O
     8    16    32
Direct
  0.1250000000000000  0.1250000000000000  0.1250000000000000
  0.6250000000000000  0.1250000000000000  0.6250000000000000
  0.1250000000000000  0.6250000000000000  0.6250000000000000
  0.6250000000000000  0.6250000000000000  0.1250000000000000
  0.8750000000000000  0.3750000000000000  0.3750000000000000
  0.8750000000000000  0.8750000000000000  0.8750000000000000
  0.3750000000000000  0.3750000000000000  0.8750000000000000
  0.3750000000000000  0.8750000000000000  0.3750000000000000
  0.5000000000000000  0.5000000000000000  0.5000000000000000
  0.2500000000000000  0.7500000000000000  0.0000000000000000
  0.7500000000000000  0.0000000000000000  0.2500000000000000
  0.0000000000000000  0.2500000000000000  0.7500000000000000
  0.7500000000000000  0.2500000000000000  0.0000000000000000
  0.2500000000000000  0.0000000000000000  0.7500000000000000
  0.0000000000000000  0.7500000000000000  0.2500000000000000
  0.5000000000000000  0.0000000000000000  0.0000000000000000
  0.2500000000000000  0.2500000000000000  0.5000000000000000
  0.7500000000000000  0.5000000000000000  0.7500000000000000
  0.7500000000000000  0.7500000000000000  0.5000000000000000
  0.2500000000000000  0.5000000000000000  0.2500000000000000
  0.0000000000000000  0.5000000000000000  0.0000000000000000
  0.5000000000000000  0.2500000000000000  0.2500000000000000
  0.5000000000000000  0.7500000000000000  0.7500000000000000
  0.0000000000000000  0.0000000000000000  0.5000000000000000
  0.2627472841061365  0.2627472841061365  0.2627472841061365
  0.4872527158938635  0.9872527158938634  0.7627472841061366
  0.9872527158938634  0.7627472841061366  0.4872527158938635
  0.7627472841061366  0.4872527158938635  0.9872527158938634
  0.0127472841061365  0.5127472841061366  0.2372527158938635
  0.7372527158938634  0.7372527158938634  0.7372527158938634
  0.5127472841061366  0.2372527158938635  0.0127472841061365
  0.2372527158938635  0.0127472841061365  0.5127472841061366
  0.5127472841061366  0.0127472841061365  0.2372527158938635
  0.0127472841061365  0.2372527158938635  0.5127472841061366
  0.2372527158938635  0.5127472841061366  0.0127472841061365
  0.9872527158938634  0.4872527158938635  0.7627472841061366
  0.4872527158938635  0.7627472841061366  0.9872527158938634
  0.7627472841061366  0.9872527158938634  0.4872527158938635
  0.2627472841061365  0.7627472841061366  0.7627472841061366
  0.4872527158938635  0.4872527158938635  0.2627472841061365
  0.9872527158938634  0.2627472841061365  0.9872527158938634
  0.0127472841061365  0.0127472841061365  0.7372527158938634
  0.7372527158938634  0.2372527158938635  0.2372527158938635
  0.5127472841061366  0.7372527158938634  0.5127472841061366
  0.5127472841061366  0.5127472841061366  0.7372527158938634
  0.0127472841061365  0.7372527158938634  0.0127472841061365
  0.9872527158938634  0.9872527158938634  0.2627472841061365
  0.4872527158938635  0.2627472841061365  0.4872527158938635
  0.7627472841061366  0.2627472841061365  0.7627472841061366
  0.2627472841061365  0.4872527158938635  0.4872527158938635
  0.2372527158938635  0.7372527158938634  0.2372527158938635
```

3. Optimised lattice geometry and ionic positions for $LiMn_{1.5}Ni_{0.5}O_4$

Format: VASP POSCAR file

```
Li Ni Mn O
   1.0000000000000000
     8.2061908316793666    0.0259489110133812    0.0000000000000000
     0.0259489110133812    8.2061908316793666    0.0000000000000000
    -0.0000000000000000   -0.0000000000000000    8.4146280562520612
   Li   Ni   Mn   O
     8     4    12    32
Direct
  0.1208566457535635  0.1214847681639917  0.1207376360905351
  0.6291433542464364  0.1285152318360083  0.6207376360905351
  0.1287343998670981  0.6245290363758530  0.6212999452454613
  0.6212656001329019  0.6254709636241470  0.1212999452454613
  0.8714847681639917  0.3708566457535635  0.3792623639094578
  0.8785152318360083  0.8791433542464364  0.8792623639094649
  0.3745290363758530  0.3787343998670981  0.8787000547545387
  0.3754709636241470  0.8712656001329019  0.3787000547545387
  0.5009602047960844  0.4990397952039228  0.5000000000000000
  0.2490397952039157  0.7509602047960844  0.0000000000000000
  0.7469006805754552  0.9969006805754552  0.2500000000000000
  0.0030993194245448  0.2530993194245448  0.7500000000000000
  0.7471693900688734  0.2528306099311267  0.0000000000000000
  0.2528200239625895  0.0025174945206890  0.7516578649458704
  0.9974825054793111  0.7471799760374105  0.2483421350541297
  0.5004609503732514  0.0025482092504695  0.9947603169566815
  0.2495390496267486  0.2474517907495305  0.4947603169566815
  0.7525174945206889  0.5028200239625895  0.7483421350541296
  0.7525482092504695  0.7504609503732514  0.5052396830433185
  0.2466956790159850  0.4966956790159850  0.2500000000000000
  0.9974517907495305  0.4995390496267486  0.0052396830433185
  0.4971799760374105  0.2474825054793110  0.2516578649458703
  0.5033043209840150  0.7533043209840150  0.7500000000000000
  0.0028306099311266  0.9971693900688734  0.5000000000000000
  0.2594366584243758  0.2578711892518081  0.2632387860462411
  0.4905633415756242  0.9921288107481918  0.7632387860462411
  0.9893271365721110  0.7569311547991920  0.4821093364024664
  0.7606728634278890  0.4930688452008080  0.9821093364024663
  0.0078711892518081  0.5094366584243758  0.2367612139537589
  0.7421288107481918  0.7405633415756242  0.7367612139537589
  0.5069311547991920  0.2393271365721110  0.0178906635975336
  0.2430688452008079  0.0106728634278961  0.5178906635975337
  0.5055918570291146  0.0090507566140311  0.2274533675383855
  0.0191372323491933  0.2328835331710633  0.4951661426746514
  0.2299453295942063  0.5003605027529520  0.0212307912301326
  0.9909492433859689  0.4944081429708854  0.7725466324616145
  0.4996394972470480  0.7700546704057937  0.9787692087698674
  0.7671164668289367  0.9808627676508067  0.5048338573253486
  0.2703903077351128  0.7685280740030340  0.7524991481922543
  0.4796096922648872  0.4814719259969660  0.2524991481922543
  0.9828835331710633  0.2691372323491933  0.0048338573253486
  0.0236448852389072  0.0154758265708955  0.7555768004382646
  0.7263551147610928  0.2345241734291045  0.2555768004382646
  0.5200546704057937  0.7496394972470480  0.5212307912301326
  0.5185280740030340  0.5203903077351127  0.7475008518077457
  0.9987147862501721  0.7326411559537384  0.0216673639060260
  0.9845241734291045  0.9763551147610928  0.2444231995617354
  0.4826411559537384  0.2487147862501720  0.4783326360939740
  0.7654758265708955  0.2736448852389072  0.7444231995617354
  0.2503605027529520  0.4799453295942134  0.4787692087698674
  0.2314719259969660  0.7296096922648873  0.2475008518077457
```