Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information: CO, NO, and SO Adsorption on Ni Nanoclusters: a DFT Investigation

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A Vibrational Frequencies

Below, we provided the vibrational frequencies (in cm^{-1}) for the lowest energy configurations of the Ni_n nanoclusters ($n = 2 - 15$). For the linear structure are shown the $3n - 5$ vibrational modes, while for non-linear structures are presented the $3n - 6$ vibrational modes, where n is the number of atoms in the nanocluster.

Ni_2

339.07

Ni_3

334.04 193.03 189.39

Ni_4

338.43 284.36 192.97 167.85 165.86 143.53

Ni_5

318.31 264.23 263.94 234.14 191.62 178.76 170.58 169.77 63.95

Ni_6

314.58 275.21 245.61 244.29 213.88 193.35 192.04 162.56 160.94 150.73 148.06 82.32

Ni_7

308.30 300.11 252.48 252.09 209.28 207.59 206.66 183.45 160.41 159.61 137.77 134.35 133.90 86.03 82.87

Ni_8

295.67 290.27 286.12 254.83 231.00 223.77 218.70 185.25 175.96 173.24 145.95 127.11 121.95 119.23 100.16 95.53 90.17 81.22

Ni_9

294.81 285.53 283.44 266.18 260.34 246.31 245.35 206.50 205.77 192.88 178.08 173.70 151.89 135.92 133.72 127.06 111.52 102.67 83.96 75.47 58.09

Ni_{10}

335.18 334.27 334.21 284.93 252.33 251.40 250.88 245.99 240.81 240.33 240.11 179.35 177.95 176.07 139.45 138.10 131.85 129.05 124.98 124.31 122.01 100.87 97.74 94.99

Ni_{11}

337.15 336.76 287.02 278.78 273.04 261.84 261.24 249.29 195.66 195.34 191.76 191.35 174.46 168.98 167.06 166.42 158.03 157.50 143.28 142.18 132.13 129.58 117.30 115.39 94.32 91.22 43.61

Ni_{12}

325.27 324.97 306.06 286.01 269.94 267.97 248.13 239.47 236.26 217.14 205.45 193.67 186.70 183.63 174.52 172.43 161.46 152.68 149.78 145.59 138.29 136.36 134.72 123.22 119.11 117.42 108.88 106.51 98.69 98.49

Ni_{13}

325.49 324.42 304.13 302.45 272.30 265.63 264.04 240.46 235.14 234.08 214.34 206.97 198.66 187.42 186.69 178.72 167.49 165.52 158.46 147.28 145.11 141.66 135.88 131.88 128.52 122.97 118.97 113.35 111.03 101.12 99.92 96.67 95.99

Ni_{14}

324.65 319.02 300.67 300.22 296.77 268.35 265.36 253.89 242.39 237.33 221.10 207.97 201.74 193.69 188.81 182.03 174.67 167.28 160.59 156.35 150.85 146.30 142.74 139.89 139.22 135.90 131.75 127.99 112.32 109.65 107.53 101.77 96.60 93.82 87.94 83.69

Ni_{15}

322.86 320.41 305.10 295.37 288.38 284.19 255.55 248.80 248.37 241.61 230.64 221.85 214.14 205.71 198.22 188.82 184.04 181.43 176.30 168.11 164.76 158.29 156.99 145.52 140.89 137.84 136.66 132.07 127.47 127.17 123.99 120.36 109.52 105.28 101.25 99.40 89.77 73.78 35.83

B Atomic Positions

Below, we provided the atomic coordinates (*xyz* positions) for the lowest energy configurations of the Ni_n nanoclusters ($n = 2 - 15$).

Ni_2

Ni 0.3367200000000000 -0.6456850000000001 0.9080750000000000

Ni -0.3367200000000000 0.6456850000000001 -0.9080750000000000

Ni_3

Ni -1.2688933333333332 -0.0410900000000000 0.4412966666666667

Ni 0.9711666666666665 -0.6251400000000001 0.6874266666666666

Ni 0.2977266666666667 0.6662300000000001 -1.1287233333333333

Ni_4

Ni -1.2924888050017618 -0.4699163284690737 0.2490422592351056

Ni 0.2504052321272106 1.2244835938378582 0.6244940190042385

Ni 0.8233500538744991 -1.0212164989933310 0.4808929318198043

Ni 0.2187335190000521 0.2666492336245465 -1.3544292100591520

Ni_5

Ni -0.1413696884446018 0.1956361235992237 1.6324045741447453

Ni -0.0354318972844556 0.4081060067368014 -1.5981830014384553

Ni -1.6377029430523464 -0.1405987660055370 -0.0635590762533926

Ni 0.3583174784450698 -1.2212175680511379 -0.0678985004374972

Ni 1.4561870503363465 0.7580742037206427 0.0972360039846016

Ni_6

Ni 0.0005160595388389 1.6384501916831180 0.0279005383983737

Ni -0.0005645458696950 -1.6384621442878675 -0.0278588223898684

Ni -1.6376836239936345 -0.0454766798172166 -0.0560895890149933

Ni 1.6376962118910399 0.0455706258323989 0.0560448977534165

Ni -0.0097361518343977 0.0188396783604734 1.6388785780699617

Ni 0.0097720502678467 -0.0189216717709151 -1.6388756028168903

Ni_7

Ni -1.3470124219715043 -0.4187997324395987 -0.3159645828084727

Ni -0.2109532483513501 1.3392365156091568 -1.3478353104217113

Ni -0.2639592442058500 -2.4217874784077189 0.1000161438046803

Ni 0.8701034719366909 -0.6856487806182034 -0.9278284434385302

Ni -0.7852025224315380 1.4933712858060790 0.8973382342751499

Ni 1.4393361356048295 1.2251716429896025 0.2836743513203643

Ni 0.2976878294187220 -0.5315434529393190 1.3105996072685215

Ni_8

Ni 0.7687345383524367 0.8740363087039036 0.8215989047638139

Ni 1.2068201623061494 -1.3860479887493291 1.1609988498194834

Ni -0.9992167219884198 0.0100591351496107 -1.0156207315536392

Ni -0.2893200486401017 -2.1176724231988651 -0.3958119124747874

Ni 0.4430223806294613 1.8062183603538671 -1.2738541270516546

Ni 1.2489924136617141 -0.3996262755671118 -1.0188689228804790

Ni -1.3688876338448033 1.7180725400391417 0.5071741128495511

Ni -1.0101450904764420 -0.5050396567312063 1.2143838265277118

Ni_9

Ni -1.6772564210662786 -0.0863150171679585 -0.5226518887892073

Ni 0.1396747280247155 1.1900458331535280 -1.2730265181547100

Ni -0.2999148375073322 -1.7308964869204875 0.0405119964160079

Ni 1.5318897781989875 -0.4708823221756351 -0.6999390958485119

Ni -0.5483636994529029 1.3672922925277238 0.9569456726515000

Ni 1.7494957223489163 1.6009855643719231 0.4032553426619891

Ni 0.8288811638804940 -0.2815312344789174 1.5241728646496639

Ni -0.2271158910831801 -0.9456246781854585 -2.2011040746311528

Ni -1.4972905433434285 -0.6430739511246966 1.7718357010444166

Ni_{10}

Ni -1.2233502637690972 -0.9677410354104410 -0.6849717877544581

Ni -0.1687438546652391 -0.8325720385831765 1.4769008009920750

Ni 1.1737482149841050 -1.1285237878436387 -0.5014648078775501

Ni -0.2057437436953844 -2.7556188502748373 0.2723686260721028

Ni 2.4142756720086105 0.6319518062089653 -1.2170483853283560

Ni -2.0963751412965390 0.9341001553624526 -1.5623211416265352

Ni 0.1687838112545563 0.8325802277549190 -1.4769565262092659

Ni -1.1737438813260468 1.1290090517936271 0.5016007644773346

Ni 1.2234252661182179 0.9682882030650823 0.6852051536441994

Ni -0.1122760796131743 1.1885262679270827 2.5066873036104589

Ni_{11}

Ni -0.0085074509864214 2.3827738378356820 -0.8668220524592627

Ni 1.5871789893540171 0.6337411116318279 -0.9032072527361805

Ni -1.1974054140414001 -2.0045430086880458 -0.9883435991967406

Ni -1.5869957758040165 -0.6337274112376559 0.9032400083555370

Ni 0.7374490522691008 -1.2315331671319942 -2.0899970021982188

Ni 2.1741639555129133 0.0075880644281057 1.3044343908049907

Ni 0.6332162321140746 -1.2943524807808195 0.2047640489701976

Ni -0.7825421188144226 0.2454890428215180 -1.2023262538022994

Ni 0.2386990393919977 -0.7649069598866447 2.4058098226685711

Ni -1.9442793678014265 1.6106714179377857 0.2347031603641838

Ni 0.1490228588055693 1.0487995530702321 0.9977447292292094

Ni_{12}

Ni 0.1517924515962932 2.1028711351600986 -1.5856179839597058

Ni 0.2338553543353523 -0.2023686962512645 -1.5478573447606347

Ni 0.2475386113474087 -2.4092788315595666 -0.9063387474233799

Ni 2.2331218046465278 0.9955488980858700 -1.4933732594299194

Ni 1.8787382139955540 -0.8660774072604589 -0.0157430062160842

Ni -1.4314077911268619 1.0343886660994350 -0.2613606534306392

Ni -1.8079065427471885 -1.2110031978391174 -0.8666570511881115

Ni 0.9073984768167449 1.2250270883734462 0.4097285441814478

Ni -0.8175764342579228 0.8845966679443080 2.0088501058406827

Ni -2.6004188642776782 -0.3976098596733788 1.1851367012999674

Ni 1.3232855510483166 -0.1323002444856911 2.2174706296022766

Ni -0.3184208313765513 -1.0237942185936717 0.8557620654841109

Ni_{13}

Ni -0.0196527269450986 2.2365514253981544 -1.4404681422095891

Ni -0.0330599161381429 -0.0772273552196303 -1.4312147603401755

Ni 0.0918379951033295 -2.2657666371074825 -0.7744926759825983

Ni 2.0020369775392570 0.9672983859865383 -1.4185049456712129

Ni 1.7413509569225010 -0.8207834223599431 0.1955342371492677

Ni -1.5672470534696430 1.1328906499958169 -0.0647850021287173

Ni -1.9962296699415241 -1.1509614806070356 -0.6586286363707945

Ni 0.7290106127926794 1.3083416044142737 0.5488698709280619

Ni -0.8864994952003009 1.0343744539271107 2.2592143603509740

Ni -2.7079773745312590 -0.1784783599437958 1.4552680286823705

Ni 1.2348854130509412 -0.0557300580390994 2.3547507175673523

Ni -0.4888717954402964 -0.8588339771027798 1.0378515846729712

Ni 1.9004160762575300 -1.2716752293421330 -2.0633946366479101

Ni_{14}

Ni 1.0197416608085970 -1.8862353118827251 -1.2177063530112964

Ni 2.5746876771250164 -0.5521482817874439 0.1126355488690614

Ni 0.0172290948184557 -0.6341761490377031 -2.9712828572897036

Ni 0.4875029824044059 -1.0778700210464454 0.9497277903926040

Ni -1.1226918200560707 -1.0147548246377163 -1.0007464565620214

Ni 0.9127228986110207 0.4833681025912462 -1.1114144493514804

Ni -1.1065799657185504 0.8818523612898055 0.4397102378663789

Ni 0.1510718874964638 2.6186006085626587 -0.3615393305408130

Ni 1.3016887429785786 1.1476470127625475 1.1383595626459559

Ni -1.0836957032368808 1.2124391838437987 -1.9079930867201949

Ni -0.6203829004493908 -2.9723342763427896 0.1143032768618664

Ni -0.4569458946984959 0.3917455077013532 2.5791162353727159

Ni -1.7474685609373584 -1.2269335960544225 1.3128966418588561

Ni -0.3268800991458107 2.6287996840378476 1.9239332396081039

Ni_{15}

Ni -2.2127696876306064 -1.3124071870025453 1.1568796156704035

Ni -0.1709377932626346 0.6901119997899396 -1.4681828570524615

Ni -0.1127241470729761 -0.7697864420725100 2.2029615204439761

Ni 1.9601607615562848 1.5456631032056123 -1.3129800738458322

Ni 1.8652203464350841 -0.8511524578537966 -1.1206926856459667

Ni -0.0851387748491153 -1.4013784570852241 -2.4423992254307096

Ni 1.7823404939551875 -1.6492751076481351 1.1007060677389919

Ni -0.1796321519324202 1.6465473675739464 2.2789835491346526

Ni 1.1749346071723981 0.5397176993686674 0.6846157219954190

Ni -0.1936683001552897 -1.4474341720632964 -0.0781313454642234

Ni 0.1759476918765994 2.4964682284347006 0.0472783409010002

Ni -2.0574090483845033 -0.7554055621655227 -1.2093795680782407

Ni -1.3634566861985320 0.7300778862919071 0.5207446408824641

Ni 1.4687712077068173 0.1912966560022440 -3.1458322203847393

Ni -2.0516385192163202 0.3469564452240199 2.7854285191352428

Below, we provided the atomic coordinates (*xyz* positions) for the lowest energy configurations of the CO, NO, and SO adsorbed on Ni_6 and Ni_{10} nanoclusters.

CO/Ni_6

Ni 0.0648037418469148 1.3218742117199240 -1.3616377055310218

Ni 0.0896242782635348 -1.8564184722912225 -0.5778148755728979

Ni -1.5585353573387626 -0.3050519370865904 -1.0619918276006044

Ni 1.7092631890187895 -0.2329182719824600 -0.8769807536962014

Ni -0.0245615101748744 0.1355953616361115 0.6792082084885892

Ni 0.1647496182629175 -0.6434329851172181 -2.5419049681035339

C -0.1719863666218735 0.6213947345371470 2.3132543389703479

O -0.2733575932566461 0.9589573585843086 3.4278675830453231

NO/Ni_6

Ni -0.2236995653714421 1.4721816863545416 -1.1690398712216390

Ni -0.1227944798958807 -1.7164889625794535 -0.8134703160889482

Ni -1.8050891891159269 -0.1361763404848051 -0.6500083733770666

Ni 1.4794819589976547 -0.0952140143097491 -1.2106524284440643

Ni 0.1135885242176698 0.0764259775043793 0.6959024139204147

Ni -0.4410012453816953 -0.3061523113317935 -2.5715477744984518

N 0.3934717596228615 0.2757682654821556 2.2822393862300210

O 0.6060422369267592 0.4296556993647249 3.4365769634797343

SO/Ni_6

Ni 0.2683117355521697 1.9945587290413043 -0.5686891548145997

Ni -0.6407100436431279 -1.0012321376780113 -0.3431298435630897

Ni -1.7796232808321593 0.9742362524758594 -0.6757435280793164

Ni 1.4758717619439459 0.0390225577504692 -0.1968224618290441

Ni -0.3551681739616155 0.6994449368406981 1.2673770207207151

Ni 0.0152615180146222 0.3234236963369443 -2.1114160997051283

S 0.9860703690203433 -0.9204721896326868 1.6486410460782492

O 0.0299861139058215 -2.1089818451345774 0.9797830211922141

CO/Ni_{10}

Ni -1.4620329769603004 -1.2856600494841630 -1.3566015990309521

Ni -0.3906662051978079 -1.0470369090908269 0.7428449134980152

Ni 0.9383467862594976 -1.4308521657311635 -1.2228453064443796

Ni -0.4087155110016297 -3.0386020424670388 -0.3567652383678105

Ni 2.1657571241493221 0.2884306550698198 -2.0545761547330148

Ni -2.3594888353062711 0.5671655502652393 -2.3199680200059749

Ni -0.0916587913606873 0.4846133924109993 -2.2567878872930036

Ni -1.3910914179445542 0.8551599266835723 -0.2490702004832231

Ni 0.9858619548143586 0.7138735476954741 -0.1618500402035704

Ni -0.1979652048035473 1.0346797705613102 1.8188515111775809

C 0.7292757045937461 1.3642013362987584 3.2682958004379432

O 1.4823773727578740 1.4940269877880186 4.1484722214483885

NO/Ni_{10}

Ni -1.2304654966937543 -0.8303023778447495 -1.0533030605660469

Ni 0.1571339896865924 -0.8420663584892484 0.8987631764026091

Ni 1.1382954032242212 -0.9410186223986164 -1.3178160573408824

Ni -0.0482197574669305 -2.6834322401051969 -0.4418100134473027

Ni 2.1977734145231067 0.8624316850636812 -2.2474690330789948

Ni -2.3063348629059712 1.0236019127546203 -1.8678122955906629

Ni -0.0591457945652151 0.9967952940722956 -2.1232570593577074

Ni -1.0827337956879222 1.2365449306443701 0.0407084189509237

Ni 1.3173325044545297 1.1032435780182346 -0.1695758740348819

Ni 0.2953583013549435 1.2012601853102087 1.9829913643389032

N 0.0711910905407842 -0.4813782538848858 2.6053065768647827

O -0.4501849964643833 -0.6456797331407135 3.6932738568592596

SO/Ni_{10}

Ni -1.6155836687819862 -0.9067073662282950 -1.1291897710459757

Ni -0.4779827557386097 -0.8706633649306916 1.0755062393518455

Ni 0.7468518697754362 -1.1483203253346712 -1.0393302260258326

Ni -0.6236865018243219 -2.7477747134376278 -0.2110979753174038

Ni 2.1108761268926499 0.5222727950827321 -1.7524953254518734

Ni -2.4034824946155360 1.0608779987258110 -1.9837261065602725

Ni -0.1223161410436776 0.9429604626312518 -1.8019475646521732

Ni -1.4613369849846976 1.0961546870720829 0.0699824539964230

Ni 1.1371524375617907 0.8084852379559564 0.2895786479263693

Ni -0.4100416601380273 1.3031846110170489 2.1204357168577985

S 0.8936876232391876 -0.2349076589898407 2.5915506528960228

O 2.2258621496577917 0.1744376364362432 1.7707332580250723