

Electronic Supplementary Information

**On the Active Site for Electrocatalytic Water Splitting on Late Transition Metals
Embedded in Graphene**

Thomas Kropp, Michael Rebarchik, and Manos Mavrikakis

*Department of Chemical and Biological Engineering, University of Wisconsin—Madison,
1415 Engineering Drive, Madison, Wisconsin 53706-1607, United States*

1. Further Equations
2. Electronic Energy of Small Organic Molecules.
3. Vibrational Data
4. HER Overpotential on Ni/GN_m-V_{2C} as a Function of the Nitrogen Content.
5. HER, OER, and ORR energetics.

*** Corresponding Authors:**

Thomas Kropp (tekropp@wisc.edu, ORCID 0000-0002-9166-566X) and

Manos Mavrikakis (emavrikakis@wisc.edu, ORCID 0000-0002-5293-5356)

1. Further Equations

Zero-point vibrational energies (E_{ZPVE}) are calculated from harmonic frequencies (ω_i) using eq. S1, and entropies (S) are calculated from partition functions (q_i) using eq. S2. For adsorbed species, only the vibrational partition function is included (q_{vib} in eq. S3), but for gas phase species, translational and rotational partition functions (q_{trans} and q_{rot} in eqs. S4 and S5, respectively) are considered as well. Herein, β is $1/k_B T$, m is the mass of the gas phase species, P is the pressure, and I is the moment of inertia for each rotation axis.

$$E_{ZPVE} = \sum \frac{\hbar \omega_i}{2} \quad (S1)$$

$$S = \frac{\partial}{\partial T} k_B T \sum \ln(q_i) \quad (S2)$$

$$q_{vib} = \prod \frac{e^{-0.5\beta\hbar\omega_i}}{1 - e^{-\beta\hbar\omega_i}} \quad (S3)$$

$$q_{trans} = \left(\frac{2\pi m}{\beta h^2} \right)^{1.5} \frac{1}{\beta P} \quad (S4)$$

$$q_{rot} = \left(\frac{8\pi}{\beta h^2} \right)^{1.5} \sqrt{I_x I_y I_z} \quad (S5)$$

2. Electronic Energy of Small Organic Molecules.

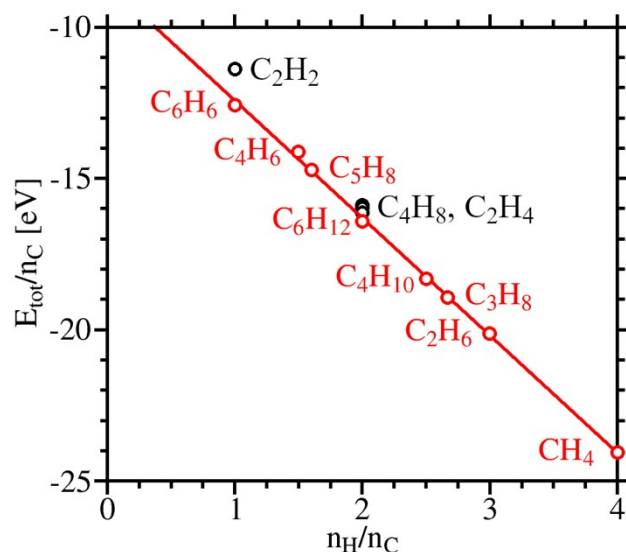


Fig. S1. Electronic energy obtained using PBE for small organic molecules divided by the number of C atoms as a function of the hydrogen-to-carbon ratio. Only the most stable molecules at a given

(n_H/n_C) ratio (red circles) were included in the fit, i.e. $y = -3.87x - 8.57$ (MAE = 0.06 eV, $R^2 = 0.99$). Less stable species (not included) in the fit are shown as black circles.

3. Vibrational Data

H on Ag/GN₃-V_{2c}

1 f = 83.405521 THz 524.052347 2PiTHz 2782.108644 cm⁻¹ 344.937634 meV
 2 f = 33.841920 THz 212.635053 2PiTHz 1128.844897 cm⁻¹ 139.958980 meV
 3 f = 26.638690 THz 167.375824 2PiTHz 888.571016 cm⁻¹ 110.168805 meV

H on Au/GN₃-V_{2c}

1 f = 62.918043 THz 395.325725 2PiTHz 2098.719954 cm⁻¹ 260.208205 meV
 2 f = 22.342936 THz 140.384807 2PiTHz 745.280098 cm⁻¹ 92.402989 meV
 3 f = 18.946991 THz 119.047454 2PiTHz 632.003563 cm⁻¹ 78.358483 meV

H on Ag/GN₄-V_{2c}

1 f = 52.493612 THz 329.827091 2PiTHz 1750.998365 cm⁻¹ 217.096207 meV
 2 f = 7.014857 THz 44.075648 2PiTHz 233.990445 cm⁻¹ 29.011128 meV
 3 f = 6.186075 THz 38.868254 2PiTHz 206.345238 cm⁻¹ 25.583558 meV

H on Au/GN₄-V_{2c}

1 f = 32.319140 THz 203.067145 2PiTHz 1078.050434 cm⁻¹ 133.661267 meV
 2 f = 11.473000 THz 72.086983 2PiTHz 382.698066 cm⁻¹ 47.448530 meV
 3 f = 10.814666 THz 67.950553 2PiTHz 360.738432 cm⁻¹ 44.725881 meV

H on Co/GN₄-V_{2c}

1 f = 61.216572 THz 384.635065 2PiTHz 2041.964979 cm⁻¹ 253.171482 meV
 2 f = 19.101941 THz 120.021036 2PiTHz 637.172150 cm⁻¹ 78.999307 meV
 3 f = 16.907973 THz 106.235926 2PiTHz 563.989246 cm⁻¹ 69.925780 meV

H on Cr/GN₄-V_{2c}

1 f = 52.696452 THz 331.101576 2PiTHz 1757.764396 cm⁻¹ 217.935088 meV
 2 f = 13.544790 THz 85.104426 2PiTHz 451.805550 cm⁻¹ 56.016769 meV
 3 f = 12.894426 THz 81.018069 2PiTHz 430.111747 cm⁻¹ 53.327079 meV

H on Cu/GN₃-V_{2C}

1 f = 82.229611 THz 516.663885 2PiTHz 2742.884504 cm-1 340.074459 meV
2 f = 33.232721 THz 208.807346 2PiTHz 1108.524226 cm-1 137.439537 meV
3 f = 25.973175 THz 163.194274 2PiTHz 866.371846 cm-1 107.416457 meV

H on Cu/GN₄-V_{2C}

1 f = 49.587980 THz 311.570470 2PiTHz 1654.076933 cm-1 205.079476 meV
2 f = 13.048601 THz 81.986781 2PiTHz 435.254480 cm-1 53.964697 meV
3 f = 12.117928 THz 76.139184 2PiTHz 404.210541 cm-1 50.115738 meV

H on Fe/GN₄-V_{2C}

1 f = 58.703965 THz 368.847890 2PiTHz 1958.153435 cm-1 242.780171 meV
2 f = 17.516960 THz 110.062303 2PiTHz 584.302857 cm-1 72.444347 meV
3 f = 13.701012 THz 86.085998 2PiTHz 457.016557 cm-1 56.662852 meV

H on Ir/GN₄-V_{2C}

1 f = 69.643295 THz 437.581725 2PiTHz 2323.050182 cm-1 288.021618 meV
2 f = 16.035269 THz 100.752567 2PiTHz 534.878985 cm-1 66.316566 meV
3 f = 11.332414 THz 71.203655 2PiTHz 378.008619 cm-1 46.867112 meV

H on Mn/GN₄-V_{2C}

1 f = 56.347447 THz 354.041450 2PiTHz 1879.548457 cm-1 233.034392 meV
2 f = 17.736134 THz 111.439414 2PiTHz 591.613717 cm-1 73.350779 meV
3 f = 16.624364 THz 104.453962 2PiTHz 554.529088 cm-1 68.752869 meV

H on Mo/GN₄-V_{2C}

1 f = 54.719725 THz 343.814175 2PiTHz 1825.253514 cm-1 226.302675 meV
2 f = 9.548781 THz 59.996763 2PiTHz 318.513051 cm-1 39.490600 meV
3 f = 8.544380 THz 53.685924 2PiTHz 285.009834 cm-1 35.336728 meV

H on Ni/GN₁-V_{2c}

1 f = 69.462434 THz 436.445348 2PiTHz 2317.017340 cm-1 287.273641 meV
2 f = 35.828868 THz 225.119416 2PiTHz 1195.122354 cm-1 148.176340 meV
3 f = 27.633871 THz 173.628729 2PiTHz 921.766673 cm-1 114.284543 meV

H on Ni/GN₂-V_{2c}

1 f = 69.631912 THz 437.510205 2PiTHz 2322.670495 cm-1 287.974543 meV
2 f = 31.866073 THz 200.220440 2PiTHz 1062.937738 cm-1 131.787531 meV
3 f = 26.945157 THz 169.301412 2PiTHz 898.793652 cm-1 111.436250 meV

H on Ni/GN₃-V_{2c}

1 f = 73.601538 THz 462.452100 2PiTHz 2455.082957 cm-1 304.391602 meV
2 f = 31.532372 THz 198.123735 2PiTHz 1051.806674 cm-1 130.407454 meV
3 f = 25.018431 THz 157.195436 2PiTHz 834.524993 cm-1 103.467949 meV

H on Ni/GN₄-V_{2c}

1 f = 51.438718 THz 323.198996 2PiTHz 1715.810883 cm-1 212.733513 meV
2 f = 16.435891 THz 103.269746 2PiTHz 548.242281 cm-1 67.973404 meV
3 f = 13.702533 THz 86.095557 2PiTHz 457.067305 cm-1 56.669144 meV

H on Pd/GN₃-V_{2c}

1 f = 81.387317 THz 511.371597 2PiTHz 2714.788608 cm-1 336.591010 meV
2 f = 32.325824 THz 203.109145 2PiTHz 1078.273404 cm-1 133.688912 meV
3 f = 19.944731 THz 125.316444 2PiTHz 665.284611 cm-1 82.484809 meV

H on Pd/GN₄-V_{2c}

1 f = 48.730959 THz 306.185645 2PiTHz 1625.489769 cm-1 201.535118 meV
2 f = 14.816412 THz 93.094259 2PiTHz 494.222276 cm-1 61.275775 meV
3 f = 11.851893 THz 74.467639 2PiTHz 395.336581 cm-1 49.015507 meV

H on Pt/GN₂-V_{2c}

1 f = 66.839073 THz 419.962282 2PiTHz 2229.511424 cm-1 276.424286 meV
2 f = 12.612535 THz 79.246892 2PiTHz 420.708858 cm-1 52.161269 meV
3 f = 9.928764 THz 62.384262 2PiTHz 331.187894 cm-1 41.062080 meV

H on Pt/GN₃-V_{2c}

1 f = 64.343131 THz 404.279817 2PiTHz 2146.255771 cm-1 266.101897 meV
2 f = 14.816663 THz 93.095838 2PiTHz 494.230660 cm-1 61.276814 meV
3 f = 7.869684 THz 49.446682 2PiTHz 262.504387 cm-1 32.546408 meV

H on Pt/GN₄-V_{2c}

1 f = 60.530506 THz 380.324385 2PiTHz 2019.080279 cm-1 250.334140 meV
2 f = 14.469355 THz 90.913637 2PiTHz 482.645708 cm-1 59.840463 meV
3 f = 10.625359 THz 66.761099 2PiTHz 354.423812 cm-1 43.942968 meV

H on Rh/GN₄-V_{2c}

1 f = 65.102551 THz 409.051392 2PiTHz 2171.587288 cm-1 269.242606 meV
2 f = 17.299300 THz 108.694708 2PiTHz 577.042519 cm-1 71.544180 meV
3 f = 14.891834 THz 93.568153 2PiTHz 496.738102 cm-1 61.587697 meV

H on Ru/GN₄-V_{2c}

1 f = 63.106302 THz 396.508590 2PiTHz 2104.999594 cm-1 260.986781 meV
2 f = 15.807298 THz 99.320186 2PiTHz 527.274705 cm-1 65.373755 meV
3 f = 13.783876 THz 86.606649 2PiTHz 459.780610 cm-1 57.005551 meV

OH on Ag/GN₃-V_{2c}

1 f = 109.559965 THz 688.385565 2PiTHz 3654.526964 cm-1 453.103759 meV
2 f = 35.370418 THz 222.238893 2PiTHz 1179.830127 cm-1 146.280345 meV
3 f = 19.074232 THz 119.846937 2PiTHz 636.247889 cm-1 78.884713 meV
4 f = 11.479570 THz 72.128264 2PiTHz 382.917219 cm-1 47.475701 meV
5 f = 8.079746 THz 50.766543 2PiTHz 269.511319 cm-1 33.415157 meV
6 f = 6.030215 THz 37.888955 2PiTHz 201.146298 cm-1 24.938971 meV

O on Ag/GN₃-V_{2c}

1 f = 31.766525 THz 199.594963 2PiTHz 1059.617183 cm-1 131.375834 meV
2 f = 10.717162 THz 67.337915 2PiTHz 357.486034 cm-1 44.322635 meV
3 f = 6.477766 THz 40.701006 2PiTHz 216.075020 cm-1 26.789898 meV

OOH on Ag/GN₃-V_{2c}

1 f = 110.322252 THz 693.175150 2PiTHz 3679.954089 cm-1 456.256322 meV
2 f = 37.991460 THz 238.707385 2PiTHz 1267.258670 cm-1 157.120107 meV
3 f = 21.238303 THz 133.444190 2PiTHz 708.433494 cm-1 87.834590 meV
4 f = 18.464982 THz 116.018901 2PiTHz 615.925469 cm-1 76.365053 meV
5 f = 9.975185 THz 62.675935 2PiTHz 332.736342 cm-1 41.254063 meV
6 f = 7.896659 THz 49.616173 2PiTHz 263.404190 cm-1 32.657969 meV
7 f = 4.278609 THz 26.883294 2PiTHz 142.719035 cm-1 17.694912 meV
8 f = 3.723947 THz 23.398249 2PiTHz 124.217494 cm-1 15.401012 meV
9 f = 2.862515 THz 17.985711 2PiTHz 95.483212 cm-1 11.838414 meV

O₂ on Ag/GN₃-V_{2c}

1 f = 42.098251 THz 264.511110 2PiTHz 1404.246447 cm-1 174.104433 meV
2 f = 3.097486 THz 19.462076 2PiTHz 103.320993 cm-1 12.810175 meV
3 f = 1.718024 THz 10.794663 2PiTHz 57.307112 cm-1 7.105179 meV
4 f = 1.310691 THz 8.235316 2PiTHz 43.719952 cm-1 5.420585 meV
5 f = 0.901765 THz 5.665957 2PiTHz 30.079646 cm-1 3.729402 meV
6 f = 0.682453 THz 4.287977 2PiTHz 22.764174 cm-1 2.822399 meV

OH on Ag/GN₄-V_{2c}

1 f = 112.137851 THz 704.582898 2PiTHz 3740.515968 cm-1 463.765040 meV
2 f = 20.948472 THz 131.623129 2PiTHz 698.765774 cm-1 86.635945 meV
3 f = 12.395002 THz 77.880097 2PiTHz 413.452764 cm-1 51.261628 meV
4 f = 3.517777 THz 22.102843 2PiTHz 117.340397 cm-1 14.548360 meV
5 f = 2.110443 THz 13.260303 2PiTHz 70.396791 cm-1 8.728093 meV
6 f = 1.511663 THz 9.498061 2PiTHz 50.423662 cm-1 6.251740 meV

O on Ag/GN₄-V₂C

1 f = 13.637393 THz 85.686267 2PiTHz 454.894448 cm-1 56.399744 meV
2 f = 2.125461 THz 13.354666 2PiTHz 70.897748 cm-1 8.790204 meV
3 f = 1.355081 THz 8.514224 2PiTHz 45.200632 cm-1 5.604166 meV

OOH on Ag/GN₄-V₂C

1 f = 108.470056 THz 681.537459 2PiTHz 3618.171484 cm-1 448.596252 meV
2 f = 38.224679 THz 240.172742 2PiTHz 1275.038012 cm-1 158.084623 meV
3 f = 25.843123 THz 162.377131 2PiTHz 862.033767 cm-1 106.878604 meV
4 f = 11.657293 THz 73.244935 2PiTHz 388.845441 cm-1 48.210708 meV
5 f = 8.604730 THz 54.065110 2PiTHz 287.022872 cm-1 35.586314 meV
6 f = 5.187193 THz 32.592095 2PiTHz 173.026132 cm-1 21.452514 meV
7 f = 2.114350 THz 13.284852 2PiTHz 70.527116 cm-1 8.744251 meV
8 f = 1.822429 THz 11.450658 2PiTHz 60.789680 cm-1 7.536962 meV
9 f = 1.149938 THz 7.225271 2PiTHz 38.357790 cm-1 4.755761 meV

O₂ on Ag/GN₄-V₂C

1 f = 41.636089 THz 261.607262 2PiTHz 1388.830392 cm-1 172.193085 meV
2 f = 2.787692 THz 17.515587 2PiTHz 92.987403 cm-1 11.528973 meV
3 f = 1.610657 THz 10.120054 2PiTHz 53.725721 cm-1 6.661143 meV
4 f = 1.380084 THz 8.671326 2PiTHz 46.034657 cm-1 5.707572 meV
5 f = 1.288583 THz 8.096408 2PiTHz 42.982514 cm-1 5.329154 meV
6 f = 1.051012 THz 6.603704 2PiTHz 35.057988 cm-1 4.346638 meV

OH on Au/GN₃-V₂C

1 f = 110.209340 THz 692.465707 2PiTHz 3676.187774 cm-1 455.789358 meV
2 f = 35.285798 THz 221.707206 2PiTHz 1177.007484 cm-1 145.930382 meV
3 f = 18.420609 THz 115.740097 2PiTHz 614.445342 cm-1 76.181541 meV
4 f = 9.597583 THz 60.303391 2PiTHz 320.140891 cm-1 39.692426 meV
5 f = 7.887545 THz 49.558904 2PiTHz 263.100160 cm-1 32.620274 meV
6 f = 6.645758 THz 41.756527 2PiTHz 221.678609 cm-1 27.484654 meV

O on Au/GN₃-V_{2C}

1 f = 27.104509 THz 170.302652 2PiTHz 904.109069 cm-1 112.095278 meV
2 f = 8.315511 THz 52.247898 2PiTHz 277.375590 cm-1 34.390203 meV
3 f = 6.260799 THz 39.337763 2PiTHz 208.837782 cm-1 25.892594 meV

OOH on Au/GN₃-V_{2C}

1 f = 109.905353 THz 690.555697 2PiTHz 3666.047842 cm-1 454.532166 meV
2 f = 37.623632 THz 236.396251 2PiTHz 1254.989234 cm-1 155.598890 meV
3 f = 22.222176 THz 139.626047 2PiTHz 741.251967 cm-1 91.903564 meV
4 f = 17.721485 THz 111.347377 2PiTHz 591.125108 cm-1 73.290199 meV
5 f = 9.324501 THz 58.587568 2PiTHz 311.031867 cm-1 38.563051 meV
6 f = 8.980369 THz 56.425320 2PiTHz 299.552844 cm-1 37.139833 meV
7 f = 6.695985 THz 42.072117 2PiTHz 223.354025 cm-1 27.692380 meV
8 f = 3.790803 THz 23.818316 2PiTHz 126.447564 cm-1 15.677506 meV
9 f = 2.548187 THz 16.010734 2PiTHz 84.998380 cm-1 10.538460 meV

O₂ on Au/GN₃-V_{2C}

1 f = 42.542279 THz 267.301020 2PiTHz 1419.057626 cm-1 175.940785 meV
2 f = 2.979339 THz 18.719739 2PiTHz 99.380047 cm-1 12.321560 meV
3 f = 1.588996 THz 9.983959 2PiTHz 53.003213 cm-1 6.571563 meV
4 f = 1.262375 THz 7.931736 2PiTHz 42.108296 cm-1 5.220765 meV
5 f = 1.186053 THz 7.452194 2PiTHz 39.562483 cm-1 4.905125 meV
6 f = 0.302536 THz 1.900892 2PiTHz 10.091528 cm-1 1.251190 meV

OH on Au/GN₄-V_{2C}

1 f = 111.553628 THz 700.912114 2PiTHz 3721.028372 cm-1 461.348885 meV
2 f = 13.792440 THz 86.660457 2PiTHz 460.066264 cm-1 57.040967 meV
3 f = 6.718897 THz 42.216074 2PiTHz 224.118269 cm-1 27.787134 meV
4 f = 3.667339 THz 23.042570 2PiTHz 122.329255 cm-1 15.166900 meV
5 f = 1.900414 THz 11.940652 2PiTHz 63.390977 cm-1 7.859482 meV
6 f = 1.688725 THz 10.610574 2PiTHz 56.329812 cm-1 6.984009 meV

O on Au/GN₄-V_{2C}

1 f =	6.180906 THz	38.835776 2PiTHz	206.172816 cm-1	25.562180 meV
2 f =	2.193450 THz	13.781853 2PiTHz	73.165617 cm-1	9.071384 meV
3 f =	1.065598 THz	6.695351 2PiTHz	35.544530 cm-1	4.406962 meV

OOH on Au/GN₄-V_{2C}

1 f =	107.546782 THz	675.736359 2PiTHz	3587.374385 cm-1	444.777897 meV
2 f =	38.784833 THz	243.692293 2PiTHz	1293.722733 cm-1	160.401234 meV
3 f =	27.512388 THz	172.865432 2PiTHz	917.714454 cm-1	113.782132 meV
4 f =	3.951919 THz	24.830637 2PiTHz	131.821814 cm-1	16.343828 meV
5 f =	3.586801 THz	22.536535 2PiTHz	119.642797 cm-1	14.833822 meV
6 f =	2.246590 THz	14.115739 2PiTHz	74.938160 cm-1	9.291151 meV
7 f =	1.209794 THz	7.601361 2PiTHz	40.354387 cm-1	5.003308 meV
8 f =	0.847891 THz	5.327457 2PiTHz	28.282602 cm-1	3.506597 meV
9 f =	0.441308 THz	2.772819 2PiTHz	14.720446 cm-1	1.825103 meV

O₂ on Au/GN₄-V_{2C}

1 f =	41.350394 THz	259.812189 2PiTHz	1379.300641 cm-1	171.011546 meV
2 f =	2.256322 THz	14.176889 2PiTHz	75.262797 cm-1	9.331401 meV
3 f =	1.506143 THz	9.463373 2PiTHz	50.239508 cm-1	6.228907 meV
4 f =	1.274690 THz	8.009115 2PiTHz	42.519090 cm-1	5.271697 meV
5 f =	0.941588 THz	5.916170 2PiTHz	31.407983 cm-1	3.894095 meV
6 f =	0.355613 THz	2.234385 2PiTHz	11.861986 cm-1	1.470699 meV

OH on Co/GN₄-V_{2C}

1 f =	111.113523 THz	698.146855 2PiTHz	3706.348061 cm-1	459.528758 meV
2 f =	26.547658 THz	166.803857 2PiTHz	885.534537 cm-1	109.792329 meV
3 f =	14.233608 THz	89.432398 2PiTHz	474.782050 cm-1	58.865493 meV
4 f =	4.481542 THz	28.158357 2PiTHz	149.488137 cm-1	18.534173 meV
5 f =	4.332320 THz	27.220772 2PiTHz	144.510649 cm-1	17.917043 meV
6 f =	3.440016 THz	21.614260 2PiTHz	114.746592 cm-1	14.226769 meV

O on Co/GN₄-V₂C

1 f = 18.731589 THz 117.694043 2PiTHz 624.818523 cm-1 77.467652 meV
2 f = 4.978025 THz 31.277854 2PiTHz 166.049038 cm-1 20.587464 meV
3 f = 4.644164 THz 29.180143 2PiTHz 154.912630 cm-1 19.206725 meV

OOH on Co/GN₄-V₂C

1 f = 108.501436 THz 681.734628 2PiTHz 3619.218219 cm-1 448.726031 meV
2 f = 38.680308 THz 243.035543 2PiTHz 1290.236156 cm-1 159.968953 meV
3 f = 25.537266 THz 160.455372 2PiTHz 851.831461 cm-1 105.613679 meV
4 f = 13.907104 THz 87.380911 2PiTHz 463.891040 cm-1 57.515179 meV
5 f = 11.450766 THz 71.947285 2PiTHz 381.956432 cm-1 47.356579 meV
6 f = 7.165780 THz 45.023923 2PiTHz 239.024684 cm-1 29.635294 meV
7 f = 3.594480 THz 22.584786 2PiTHz 119.898954 cm-1 14.865581 meV
8 f = 2.799065 THz 17.587045 2PiTHz 93.366759 cm-1 11.576007 meV
9 f = 1.644222 THz 10.330954 2PiTHz 54.845355 cm-1 6.799960 meV

O₂ on Co/GN₄-V₂C

1 f = 37.028955 THz 232.659783 2PiTHz 1235.152935 cm-1 153.139501 meV
2 f = 13.869816 THz 87.146627 2PiTHz 462.647265 cm-1 57.360971 meV
3 f = 7.348402 THz 46.171369 2PiTHz 245.116287 cm-1 30.390557 meV
4 f = 4.340260 THz 27.270655 2PiTHz 144.775470 cm-1 17.949877 meV
5 f = 2.255855 THz 14.173957 2PiTHz 75.247233 cm-1 9.329471 meV
6 f = 2.071247 THz 13.014026 2PiTHz 69.089347 cm-1 8.565990 meV

OH on Cr/GN₄-V₂C

1 f = 111.545553 THz 700.861378 2PiTHz 3720.759023 cm-1 461.315490 meV
2 f = 21.417226 THz 134.568402 2PiTHz 714.401752 cm-1 88.574560 meV
3 f = 16.150718 THz 101.477956 2PiTHz 538.729959 cm-1 66.794026 meV
4 f = 6.332229 THz 39.786569 2PiTHz 211.220420 cm-1 26.188004 meV
5 f = 3.760519 THz 23.628036 2PiTHz 125.437397 cm-1 15.552261 meV
6 f = 3.525662 THz 22.152386 2PiTHz 117.603415 cm-1 14.580970 meV

O on Cr/GN₄-V_{2C}

1 f = 28.105153 THz 176.589885 2PiTHz 937.486970 cm-1 116.233612 meV
2 f = 5.916412 THz 37.173911 2PiTHz 197.350247 cm-1 24.468321 meV
3 f = 5.381151 THz 33.810767 2PiTHz 179.495863 cm-1 22.254659 meV

OOH on Cr/GN₄-V_{2C}

1 f = 109.973545 THz 690.984164 2PiTHz 3668.322502 cm-1 454.814188 meV
2 f = 37.707420 THz 236.922709 2PiTHz 1257.784116 cm-1 155.945411 meV
3 f = 22.441806 THz 141.006028 2PiTHz 748.578061 cm-1 92.811884 meV
4 f = 14.541700 THz 91.368195 2PiTHz 485.058883 cm-1 60.139658 meV
5 f = 6.684949 THz 42.002774 2PiTHz 222.985892 cm-1 27.646737 meV
6 f = 5.311444 THz 33.372787 2PiTHz 177.170696 cm-1 21.966375 meV
7 f = 3.056672 THz 19.205634 2PiTHz 101.959588 cm-1 12.641382 meV
8 f = 2.108194 THz 13.246176 2PiTHz 70.321791 cm-1 8.718794 meV
9 f = 2.061820 THz 12.954797 2PiTHz 68.774911 cm-1 8.527005 meV

O₂ on Cr/GN₄-V_{2C}

1 f = 27.143429 THz 170.547195 2PiTHz 905.407310 cm-1 112.256240 meV
2 f = 12.906448 THz 81.093606 2PiTHz 430.512761 cm-1 53.376799 meV
3 f = 11.311456 THz 71.071974 2PiTHz 377.309548 cm-1 46.780439 meV
4 f = 4.580054 THz 28.777328 2PiTHz 152.774154 cm-1 18.941588 meV
5 f = 4.294607 THz 26.983810 2PiTHz 143.252656 cm-1 17.761072 meV
6 f = 2.790626 THz 17.534019 2PiTHz 93.085253 cm-1 11.541105 meV

OH on Cu/GN₃-V_{2C}

1 f = 109.990645 THz 691.091604 2PiTHz 3668.892881 cm-1 454.884906 meV
2 f = 35.317469 THz 221.906203 2PiTHz 1178.063929 cm-1 146.061364 meV
3 f = 18.470259 THz 116.052063 2PiTHz 616.101519 cm-1 76.386880 meV
4 f = 10.870118 THz 68.298964 2PiTHz 362.588089 cm-1 44.955210 meV
5 f = 8.097350 THz 50.877150 2PiTHz 270.098510 cm-1 33.487959 meV
6 f = 6.206807 THz 38.998518 2PiTHz 207.036788 cm-1 25.669299 meV

O on Cu/GN₃-V_{2c}

1 f = 27.193456 THz 170.861521 2PiTHz 907.076018 cm-1 112.463133 meV
2 f = 9.983459 THz 62.727924 2PiTHz 333.012342 cm-1 41.288283 meV
3 f = 6.845958 THz 43.014424 2PiTHz 228.356576 cm-1 28.312617 meV

OOH on Cu/GN₃-V_{2c}

1 f = 110.284964 THz 692.940865 2PiTHz 3678.710309 cm-1 456.102112 meV
2 f = 37.700901 THz 236.881744 2PiTHz 1257.566638 cm-1 155.918448 meV
3 f = 19.869568 THz 124.844178 2PiTHz 662.777431 cm-1 82.173958 meV
4 f = 17.314237 THz 108.788558 2PiTHz 577.540752 cm-1 71.605953 meV
5 f = 9.640540 THz 60.573301 2PiTHz 321.573800 cm-1 39.870084 meV
6 f = 8.097777 THz 50.879831 2PiTHz 270.112742 cm-1 33.489724 meV
7 f = 5.304612 THz 33.329859 2PiTHz 176.942798 cm-1 21.938119 meV
8 f = 4.348069 THz 27.319722 2PiTHz 145.035960 cm-1 17.982174 meV
9 f = 2.312427 THz 14.529404 2PiTHz 77.134244 cm-1 9.563431 meV

O₂ on Cu/GN₃-V_{2c}

1 f = 42.237884 THz 265.388451 2PiTHz 1408.904104 cm-1 174.681909 meV
2 f = 4.027945 THz 25.308328 2PiTHz 134.357795 cm-1 16.658249 meV
3 f = 1.917136 THz 12.045718 2PiTHz 63.948757 cm-1 7.928638 meV
4 f = 1.845680 THz 11.596752 2PiTHz 61.565267 cm-1 7.633123 meV
5 f = 1.251025 THz 7.860422 2PiTHz 41.729700 cm-1 5.173825 meV
6 f = 0.669308 THz 4.205386 2PiTHz 22.325710 cm-1 2.768036 meV

OH on Cu/GN₄-V_{2c}

1 f = 112.146790 THz 704.639066 2PiTHz 3740.814154 cm-1 463.802011 meV
2 f = 21.222774 THz 133.346623 2PiTHz 707.915525 cm-1 87.770370 meV
3 f = 11.716672 THz 73.618020 2PiTHz 390.826093 cm-1 48.456277 meV
4 f = 5.313944 THz 33.388495 2PiTHz 177.254086 cm-1 21.976714 meV
5 f = 2.994500 THz 18.814999 2PiTHz 99.885768 cm-1 12.384261 meV
6 f = 2.466913 THz 15.500072 2PiTHz 82.287363 cm-1 10.202336 meV

O on Cu/GN₄-V₂C

1 f = 17.551513 THz 110.279406 2PiTHz 585.455426 cm-1 72.587248 meV
2 f = 3.295391 THz 20.705551 2PiTHz 109.922401 cm-1 13.628646 meV
3 f = 2.396592 THz 15.058232 2PiTHz 79.941706 cm-1 9.911512 meV

OOH on Cu/GN₄-V₂C

1 f = 108.298491 THz 680.459486 2PiTHz 3612.448701 cm-1 447.886717 meV
2 f = 38.753521 THz 243.495552 2PiTHz 1292.678266 cm-1 160.271736 meV
3 f = 26.422706 THz 166.018756 2PiTHz 881.366563 cm-1 109.275566 meV
4 f = 9.077554 THz 57.035953 2PiTHz 302.794592 cm-1 37.541758 meV
5 f = 8.199419 THz 51.518469 2PiTHz 273.503168 cm-1 33.910083 meV
6 f = 4.540942 THz 28.531580 2PiTHz 151.469516 cm-1 18.779833 meV
7 f = 2.064881 THz 12.974032 2PiTHz 68.877025 cm-1 8.539666 meV
8 f = 1.625145 THz 10.211084 2PiTHz 54.208984 cm-1 6.721060 meV
9 f = 1.311292 THz 8.239092 2PiTHz 43.739998 cm-1 5.423070 meV

O₂ on Cu/GN₄-V₂C

1 f = 42.285010 THz 265.684552 2PiTHz 1410.476060 cm-1 174.876806 meV
2 f = 3.310304 THz 20.799256 2PiTHz 110.419868 cm-1 13.690324 meV
3 f = 1.197294 THz 7.522820 2PiTHz 39.937428 cm-1 4.951612 meV
4 f = 1.146930 THz 7.206371 2PiTHz 38.257453 cm-1 4.743321 meV
5 f = 0.753062 THz 4.731629 2PiTHz 25.119450 cm-1 3.114416 meV
6 f = 0.530694 THz 3.334447 2PiTHz 17.702035 cm-1 2.194773 meV

OH on Fe/GN₄-V₂C

1 f = 110.162517 THz 692.171505 2PiTHz 3674.625903 cm-1 455.595711 meV
2 f = 25.790014 THz 162.043435 2PiTHz 860.262232 cm-1 106.658962 meV
3 f = 15.697389 THz 98.629605 2PiTHz 523.608524 cm-1 64.919206 meV
4 f = 8.777344 THz 55.149679 2PiTHz 292.780675 cm-1 36.300190 meV
5 f = 4.293628 THz 26.977660 2PiTHz 143.220008 cm-1 17.757024 meV
6 f = 3.983602 THz 25.029707 2PiTHz 132.878644 cm-1 16.474858 meV

O on Fe/GN₄-V₂C

1 f = 22.955617 THz 144.234398 2PiTHz 765.716950 cm-1 94.936836 meV
2 f = 5.358714 THz 33.669793 2PiTHz 178.747451 cm-1 22.161867 meV
3 f = 5.026518 THz 31.582544 2PiTHz 167.666586 cm-1 20.788015 meV

OOH on Fe/GN₄-V₂C

1 f = 109.739777 THz 689.515352 2PiTHz 3660.524816 cm-1 453.847398 meV
2 f = 36.799668 THz 231.219132 2PiTHz 1227.504751 cm-1 152.191247 meV
3 f = 20.571104 THz 129.252057 2PiTHz 686.178142 cm-1 85.075277 meV
4 f = 14.887173 THz 93.538865 2PiTHz 496.582616 cm-1 61.568420 meV
5 f = 7.597351 THz 47.735563 2PiTHz 253.420337 cm-1 31.420129 meV
6 f = 6.464375 THz 40.616864 2PiTHz 215.628322 cm-1 26.734514 meV
7 f = 4.893360 THz 30.745885 2PiTHz 163.224903 cm-1 20.237316 meV
8 f = 2.804025 THz 17.618209 2PiTHz 93.532208 cm-1 11.596520 meV
9 f = 2.724784 THz 17.120325 2PiTHz 90.889018 cm-1 11.268806 meV

O₂ on Fe/GN₄-V₂C

1 f = 36.071178 THz 226.641893 2PiTHz 1203.204937 cm-1 149.178453 meV
2 f = 17.055063 THz 107.160124 2PiTHz 568.895662 cm-1 70.534098 meV
3 f = 8.987066 THz 56.467400 2PiTHz 299.776238 cm-1 37.167530 meV
4 f = 7.066339 THz 44.399115 2PiTHz 235.707679 cm-1 29.224038 meV
5 f = 2.890640 THz 18.162428 2PiTHz 96.421374 cm-1 11.954731 meV
6 f = 2.733494 THz 17.175048 2PiTHz 91.179534 cm-1 11.304825 meV

OH on Ir/GN₄-V₂C

1 f = 110.756910 THz 695.906188 2PiTHz 3694.452727 cm-1 458.053924 meV
2 f = 29.032120 THz 182.414192 2PiTHz 968.407263 cm-1 120.067241 meV
3 f = 15.183324 THz 95.399635 2PiTHz 506.461142 cm-1 62.793201 meV
4 f = 5.689798 THz 35.750057 2PiTHz 189.791237 cm-1 23.531123 meV
5 f = 2.558113 THz 16.073095 2PiTHz 85.329448 cm-1 10.579507 meV
6 f = 2.243922 THz 14.098978 2PiTHz 74.849179 cm-1 9.280119 meV

O on Ir/GN₄-V_{2C}

1 f = 20.629103 THz 129.616478 2PiTHz 688.112795 cm-1 85.315144 meV
2 f = 3.929322 THz 24.688657 2PiTHz 131.068065 cm-1 16.250375 meV
3 f = 3.531962 THz 22.191971 2PiTHz 117.813564 cm-1 14.607025 meV

OOH on Ir/GN₄-V_{2C}

1 f = 109.183765 THz 686.021829 2PiTHz 3641.978271 cm-1 451.547919 meV
2 f = 37.873966 THz 237.969147 2PiTHz 1263.339482 cm-1 156.634189 meV
3 f = 21.953519 THz 137.938030 2PiTHz 732.290558 cm-1 90.792490 meV
4 f = 14.575550 THz 91.580882 2PiTHz 486.188000 cm-1 60.279651 meV
5 f = 10.584125 THz 66.502020 2PiTHz 353.048404 cm-1 43.772439 meV
6 f = 6.937336 THz 43.588565 2PiTHz 231.404602 cm-1 28.690524 meV
7 f = 3.633641 THz 22.830839 2PiTHz 121.205210 cm-1 15.027536 meV
8 f = 1.839950 THz 11.560750 2PiTHz 61.374139 cm-1 7.609426 meV
9 f = 1.460982 THz 9.179620 2PiTHz 48.733108 cm-1 6.042138 meV

O₂ on Ir/GN₄-V_{2C}

1 f = 35.735639 THz 224.533642 2PiTHz 1192.012574 cm-1 147.790777 meV
2 f = 14.672459 THz 92.189782 2PiTHz 489.420551 cm-1 60.680436 meV
3 f = 7.648958 THz 48.059824 2PiTHz 255.141784 cm-1 31.633561 meV
4 f = 4.100859 THz 25.766454 2PiTHz 136.789912 cm-1 16.959794 meV
5 f = 1.622757 THz 10.196082 2PiTHz 54.129342 cm-1 6.711185 meV
6 f = 1.235002 THz 7.759744 2PiTHz 41.195217 cm-1 5.107558 meV

OH on Mn/GN₄-V_{2C}

1 f = 111.611306 THz 701.274520 2PiTHz 3722.952328 cm-1 461.587426 meV
2 f = 21.807644 THz 137.021467 2PiTHz 727.424677 cm-1 90.189198 meV
3 f = 16.126402 THz 101.325174 2PiTHz 537.918865 cm-1 66.693463 meV
4 f = 5.758194 THz 36.179802 2PiTHz 192.072682 cm-1 23.813986 meV
5 f = 4.060906 THz 25.515427 2PiTHz 135.457252 cm-1 16.794565 meV
6 f = 3.223371 THz 20.253038 2PiTHz 107.520083 cm-1 13.330796 meV

O on Mn/GN₄-V_{2c}

1 f = 25.571428 THz 160.670019 2PiTHz 852.970987 cm-1 105.754962 meV
2 f = 5.618735 THz 35.303556 2PiTHz 187.420835 cm-1 23.237230 meV
3 f = 5.111506 THz 32.116542 2PiTHz 170.501498 cm-1 21.139499 meV

OOH on Mn/GN₄-V_{2c}

1 f = 109.740964 THz 689.522815 2PiTHz 3660.564435 cm-1 453.852310 meV
2 f = 37.105680 THz 233.141864 2PiTHz 1237.712221 cm-1 153.456813 meV
3 f = 20.805699 THz 130.726065 2PiTHz 694.003410 cm-1 86.045487 meV
4 f = 14.509440 THz 91.165503 2PiTHz 483.982824 cm-1 60.006244 meV
5 f = 8.074447 THz 50.733248 2PiTHz 269.334557 cm-1 33.393241 meV
6 f = 6.748998 THz 42.405205 2PiTHz 225.122333 cm-1 27.911622 meV
7 f = 4.053943 THz 25.471678 2PiTHz 135.224992 cm-1 16.765768 meV
8 f = 2.474038 THz 15.544842 2PiTHz 82.525037 cm-1 10.231804 meV
9 f = 2.168141 THz 13.622829 2PiTHz 72.321384 cm-1 8.966712 meV

O₂ on Mn/GN₄-V_{2c}

1 f = 30.096739 THz 189.103388 2PiTHz 1003.919121 cm-1 124.470152 meV
2 f = 13.960543 THz 87.716680 2PiTHz 465.673584 cm-1 57.736187 meV
3 f = 13.316269 THz 83.668586 2PiTHz 444.182909 cm-1 55.071682 meV
4 f = 6.160310 THz 38.706370 2PiTHz 205.485821 cm-1 25.477004 meV
5 f = 4.302872 THz 27.035740 2PiTHz 143.528344 cm-1 17.795253 meV
6 f = 3.268097 THz 20.534059 2PiTHz 109.011980 cm-1 13.515768 meV

OH on Mo/GN₄-V_{2c}

1 f = 113.132364 THz 710.831608 2PiTHz 3773.689352 cm-1 467.878017 meV
2 f = 19.294002 THz 121.227792 2PiTHz 643.578624 cm-1 79.793608 meV
3 f = 11.061761 THz 69.503091 2PiTHz 368.980603 cm-1 45.747781 meV
4 f = 7.702366 THz 48.395394 2PiTHz 256.923272 cm-1 31.854437 meV
5 f = 3.778800 THz 23.742904 2PiTHz 126.047212 cm-1 15.627868 meV
6 f = 3.306713 THz 20.776689 2PiTHz 110.300060 cm-1 13.675469 meV

O on Mo/GN₄-V₂C

1 f = 26.917905 THz 169.130183 2PiTHz 897.884623 cm-1 111.323545 meV
2 f = 4.977416 THz 31.274025 2PiTHz 166.028711 cm-1 20.584944 meV
3 f = 4.880348 THz 30.664128 2PiTHz 162.790866 cm-1 20.183502 meV

OOH on Mo/GN₄-V₂C

1 f = 111.984815 THz 703.621346 2PiTHz 3735.411242 cm-1 463.132135 meV
2 f = 24.855363 THz 156.170849 2PiTHz 829.085627 cm-1 102.793554 meV
3 f = 23.622969 THz 148.427489 2PiTHz 787.977387 cm-1 97.696780 meV
4 f = 15.628087 THz 98.194164 2PiTHz 521.296839 cm-1 64.632594 meV
5 f = 14.070885 THz 88.409975 2PiTHz 469.354171 cm-1 58.192522 meV
6 f = 8.797124 THz 55.273963 2PiTHz 293.440474 cm-1 36.381995 meV
7 f = 6.161303 THz 38.712612 2PiTHz 205.518956 cm-1 25.481112 meV
8 f = 5.035667 THz 31.640031 2PiTHz 167.971777 cm-1 20.825854 meV
9 f = 3.595486 THz 22.591107 2PiTHz 119.932509 cm-1 14.869741 meV

O₂ on Mo/GN₄-V₂C

1 f = 26.767536 THz 168.185388 2PiTHz 892.868859 cm-1 110.701669 meV
2 f = 16.404679 THz 103.073638 2PiTHz 547.201175 cm-1 67.844323 meV
3 f = 14.785606 THz 92.900700 2PiTHz 493.194704 cm-1 61.148372 meV
4 f = 3.697663 THz 23.233104 2PiTHz 123.340770 cm-1 15.292312 meV
5 f = 3.064610 THz 19.255511 2PiTHz 102.224376 cm-1 12.674212 meV
6 f = 2.084476 THz 13.097147 2PiTHz 69.530620 cm-1 8.620701 meV

OH on Ni/GN₃-V₂C

1 f = 110.561191 THz 694.676450 2PiTHz 3687.924249 cm-1 457.244496 meV
2 f = 34.655623 THz 217.747704 2PiTHz 1155.987134 cm-1 143.324190 meV
3 f = 17.449806 THz 109.640362 2PiTHz 582.062841 cm-1 72.166621 meV
4 f = 8.237550 THz 51.758050 2PiTHz 274.775068 cm-1 34.067779 meV
5 f = 6.995179 THz 43.952006 2PiTHz 233.334048 cm-1 28.929745 meV
6 f = 5.845445 THz 36.728017 2PiTHz 194.983064 cm-1 24.174828 meV

O on Ni/GN₃-V_{2c}

1 f = 24.974977 THz 156.922406 2PiTHz 833.075521 cm-1 103.288238 meV
2 f = 11.553979 THz 72.595792 2PiTHz 385.399247 cm-1 47.783434 meV
3 f = 9.928330 THz 62.381537 2PiTHz 331.173428 cm-1 41.060287 meV

OOH on Ni/GN₃-V_{2c}

1 f = 111.188679 THz 698.619075 2PiTHz 3708.855000 cm-1 459.839579 meV
2 f = 30.584849 THz 192.170276 2PiTHz 1020.200727 cm-1 126.488815 meV
3 f = 20.911793 THz 131.392668 2PiTHz 697.542296 cm-1 86.484253 meV
4 f = 10.349756 THz 65.029436 2PiTHz 345.230695 cm-1 42.803166 meV
5 f = 9.176681 THz 57.658789 2PiTHz 306.101128 cm-1 37.951717 meV
6 f = 8.441758 THz 53.041133 2PiTHz 281.586743 cm-1 34.912319 meV
7 f = 4.012800 THz 25.213165 2PiTHz 133.852590 cm-1 16.595612 meV
8 f = 2.594859 THz 16.303978 2PiTHz 86.555165 cm-1 10.731477 meV
9 f = 2.484821 THz 15.612590 2PiTHz 82.884701 cm-1 10.276397 meV

O₂ on Ni/GN₃-V_{2c}

1 f = 38.765678 THz 243.571940 2PiTHz 1293.083802 cm-1 160.322016 meV
2 f = 9.510597 THz 59.756842 2PiTHz 317.239352 cm-1 39.332681 meV
3 f = 4.492096 THz 28.224669 2PiTHz 149.840175 cm-1 18.577821 meV
4 f = 3.342170 THz 20.999471 2PiTHz 111.482773 cm-1 13.822107 meV
5 f = 1.675583 THz 10.527997 2PiTHz 55.891421 cm-1 6.929656 meV
6 f = 1.429843 THz 8.983968 2PiTHz 47.694425 cm-1 5.913357 meV

OH on Ni/GN₄-V_{2c}

1 f = 111.421435 THz 700.081525 2PiTHz 3716.618910 cm-1 460.802182 meV
2 f = 22.188907 THz 139.417013 2PiTHz 740.142238 cm-1 91.765975 meV
3 f = 10.619465 THz 66.724064 2PiTHz 354.227199 cm-1 43.918591 meV
4 f = 4.630733 THz 29.095754 2PiTHz 154.464623 cm-1 19.151179 meV
5 f = 3.715995 THz 23.348283 2PiTHz 123.952238 cm-1 15.368124 meV
6 f = 2.425715 THz 15.241218 2PiTHz 80.913145 cm-1 10.031955 meV

O on Ni/GN₄-V₂C

1 f = 11.259634 THz 70.746369 2PiTHz 375.580962 cm-1 46.566121 meV
2 f = 3.621736 THz 22.756038 2PiTHz 120.808103 cm-1 14.978301 meV
3 f = 3.224643 THz 20.261031 2PiTHz 107.562519 cm-1 13.336057 meV

OOH on Ni/GN₄-V₂C

1 f = 107.920009 THz 678.081413 2PiTHz 3599.823896 cm-1 446.321440 meV
2 f = 38.892809 THz 244.370724 2PiTHz 1297.324413 cm-1 160.847785 meV
3 f = 26.829955 THz 168.577576 2PiTHz 894.950924 cm-1 110.959813 meV
4 f = 10.669296 THz 67.037166 2PiTHz 355.889407 cm-1 44.124679 meV
5 f = 8.760757 THz 55.045458 2PiTHz 292.227383 cm-1 36.231591 meV
6 f = 4.521100 THz 28.406910 2PiTHz 150.807664 cm-1 18.697774 meV
7 f = 2.441002 THz 15.337267 2PiTHz 81.423058 cm-1 10.095176 meV
8 f = 1.665033 THz 10.461710 2PiTHz 55.539517 cm-1 6.886025 meV
9 f = 1.426006 THz 8.959862 2PiTHz 47.566448 cm-1 5.897490 meV

O₂ on Ni/GN₄-V₂C

1 f = 43.181895 THz 271.319848 2PiTHz 1440.392927 cm-1 178.586026 meV
2 f = 2.795112 THz 17.562209 2PiTHz 93.234909 cm-1 11.559660 meV
3 f = 1.025837 THz 6.445522 2PiTHz 34.218227 cm-1 4.242521 meV
4 f = 0.994287 THz 6.247288 2PiTHz 33.165833 cm-1 4.112041 meV
5 f = 0.849632 THz 5.338398 2PiTHz 28.340684 cm-1 3.513798 meV
6 f = 0.377235 THz 2.370238 2PiTHz 12.583209 cm-1 1.560120 meV

OH on Pd/GN₃-V₂C

1 f = 110.895629 THz 696.777786 2PiTHz 3699.079900 cm-1 458.627621 meV
2 f = 34.597899 THz 217.385009 2PiTHz 1154.061643 cm-1 143.085459 meV
3 f = 17.868984 THz 112.274139 2PiTHz 596.045138 cm-1 73.900205 meV
4 f = 7.934026 THz 49.850953 2PiTHz 264.650600 cm-1 32.812504 meV
5 f = 7.377004 THz 46.351082 2PiTHz 246.070351 cm-1 30.508846 meV
6 f = 5.881830 THz 36.956630 2PiTHz 196.196737 cm-1 24.325304 meV

O on Pd/GN₃-V_{2C}

1 f = 26.037382 THz 163.597696 2PiTHz 868.513552 cm-1 107.681995 meV
2 f = 14.028280 THz 88.142281 2PiTHz 467.933031 cm-1 58.016323 meV
3 f = 10.168192 THz 63.888637 2PiTHz 339.174380 cm-1 42.052279 meV

OOH on Pd/GN₃-V_{2C}

1 f = 111.206666 THz 698.732087 2PiTHz 3709.454963 cm-1 459.913965 meV
2 f = 33.977684 THz 213.488085 2PiTHz 1133.373507 cm-1 140.520456 meV
3 f = 20.722471 THz 130.203128 2PiTHz 691.227221 cm-1 85.701284 meV
4 f = 13.436197 THz 84.422118 2PiTHz 448.183289 cm-1 55.567666 meV
5 f = 9.399390 THz 59.058108 2PiTHz 313.529885 cm-1 38.872765 meV
6 f = 9.008209 THz 56.600244 2PiTHz 300.481486 cm-1 37.254970 meV
7 f = 4.835999 THz 30.385475 2PiTHz 161.311545 cm-1 20.000090 meV
8 f = 3.261787 THz 20.494412 2PiTHz 108.801497 cm-1 13.489671 meV
9 f = 2.462268 THz 15.470883 2PiTHz 82.132403 cm-1 10.183124 meV

O₂ on Pd/GN₃-V_{2C}

1 f = 43.104415 THz 270.833029 2PiTHz 1437.808487 cm-1 178.265597 meV
2 f = 2.618572 THz 16.452973 2PiTHz 87.346155 cm-1 10.829547 meV
3 f = 1.434768 THz 9.014914 2PiTHz 47.858710 cm-1 5.933726 meV
4 f = 1.304217 THz 8.194635 2PiTHz 43.503983 cm-1 5.393808 meV
5 f = 1.097756 THz 6.897407 2PiTHz 36.617209 cm-1 4.539957 meV
6 f = 0.564476 THz 3.546707 2PiTHz 18.828889 cm-1 2.334486 meV

OH on Pd/GN₄-V_{2C}

1 f = 111.020579 THz 697.562869 2PiTHz 3703.247777 cm-1 459.144372 meV
2 f = 20.350672 THz 127.867045 2PiTHz 678.825338 cm-1 84.163646 meV
3 f = 8.222456 THz 51.663215 2PiTHz 274.271605 cm-1 34.005357 meV
4 f = 4.324536 THz 27.171860 2PiTHz 144.250985 cm-1 17.884849 meV
5 f = 2.442578 THz 15.347173 2PiTHz 81.475644 cm-1 10.101696 meV
6 f = 1.728988 THz 10.863555 2PiTHz 57.672845 cm-1 7.150524 meV

O on Pd/GN₄-V₂C

1 f =	13.657121 THz	85.810219 2PiTHz	455.552491 cm-1	56.481331 meV
2 f =	2.863981 THz	17.994923 2PiTHz	95.532119 cm-1	11.844477 meV
3 f =	2.727897 THz	17.139885 2PiTHz	90.992860 cm-1	11.281681 meV

OOH on Pd/GN₄-V₂C

1 f =	106.550007 THz	669.473437 2PiTHz	3554.125551 cm-1	440.655566 meV
2 f =	39.679017 THz	249.310619 2PiTHz	1323.549515 cm-1	164.099285 meV
3 f =	28.502128 THz	179.084155 2PiTHz	950.728639 cm-1	117.875371 meV
4 f =	10.085305 THz	63.367841 2PiTHz	336.409559 cm-1	41.709484 meV
5 f =	5.419246 THz	34.050125 2PiTHz	180.766573 cm-1	22.412207 meV
6 f =	2.879581 THz	18.092944 2PiTHz	96.052496 cm-1	11.908996 meV
7 f =	1.602723 THz	10.070205 2PiTHz	53.461080 cm-1	6.628332 meV
8 f =	1.451934 THz	9.122772 2PiTHz	48.431314 cm-1	6.004720 meV
9 f =	1.025962 THz	6.446312 2PiTHz	34.222423 cm-1	4.243041 meV

O₂ on Pd/GN₄-V₂C

1 f =	43.304108 THz	272.087734 2PiTHz	1444.469511 cm-1	179.091459 meV
2 f =	2.676681 THz	16.818085 2PiTHz	89.284478 cm-1	11.069868 meV
3 f =	1.652993 THz	10.386062 2PiTHz	55.137914 cm-1	6.836232 meV
4 f =	0.906379 THz	5.694944 2PiTHz	30.233533 cm-1	3.748482 meV
5 f =	0.714268 THz	4.487881 2PiTHz	23.825430 cm-1	2.953978 meV
6 f =	0.550870 THz	3.461215 2PiTHz	18.375028 cm-1	2.278214 meV

OH on Pt/GN₃-V₂C

1 f =	111.184308 THz	698.591608 2PiTHz	3708.709186 cm-1	459.821501 meV
2 f =	33.875556 THz	212.846397 2PiTHz	1129.966889 cm-1	140.098089 meV
3 f =	17.383082 THz	109.221124 2PiTHz	579.837178 cm-1	71.890674 meV
4 f =	8.072066 THz	50.718284 2PiTHz	269.255119 cm-1	33.383392 meV
5 f =	6.614152 THz	41.557943 2PiTHz	220.624360 cm-1	27.353944 meV
6 f =	4.895013 THz	30.756274 2PiTHz	163.280052 cm-1	20.244154 meV

O on Pt/GN₃-V_{2C}

1 f = 24.808109 THz 155.873946 2PiTHz 827.509419 cm-1 102.598129 meV
2 f = 15.129148 THz 95.059242 2PiTHz 504.654051 cm-1 62.569150 meV
3 f = 10.072916 THz 63.289997 2PiTHz 335.996296 cm-1 41.658246 meV

OOH on Pt/GN₃-V_{2C}

1 f = 110.907548 THz 696.852675 2PiTHz 3699.477469 cm-1 458.676913 meV
2 f = 35.803872 THz 224.962362 2PiTHz 1194.288577 cm-1 148.072965 meV
3 f = 20.591470 THz 129.380021 2PiTHz 686.857483 cm-1 85.159505 meV
4 f = 16.565617 THz 104.084844 2PiTHz 552.569503 cm-1 68.509912 meV
5 f = 9.319338 THz 58.555127 2PiTHz 310.859643 cm-1 38.541697 meV
6 f = 8.937585 THz 56.156503 2PiTHz 298.125735 cm-1 36.962894 meV
7 f = 5.447371 THz 34.226842 2PiTHz 181.704734 cm-1 22.528524 meV
8 f = 3.705538 THz 23.282583 2PiTHz 123.603445 cm-1 15.324880 meV
9 f = 2.995870 THz 18.823605 2PiTHz 99.931458 cm-1 12.389926 meV

O₂ on Pt/GN₃-V_{2C}

1 f = 43.415804 THz 272.789541 2PiTHz 1448.195291 cm-1 179.553397 meV
2 f = 2.274749 THz 14.292667 2PiTHz 75.877446 cm-1 9.407608 meV
3 f = 1.366710 THz 8.587294 2PiTHz 45.588544 cm-1 5.652261 meV
4 f = 1.102298 THz 6.925942 2PiTHz 36.768699 cm-1 4.558739 meV
5 f = 0.921055 THz 5.787158 2PiTHz 30.723080 cm-1 3.809178 meV
6 f = 0.419062 THz 2.633047 2PiTHz 13.978417 cm-1 1.733103 meV

OH on Pt/GN₄-V_{2C}

1 f = 110.971032 THz 697.251561 2PiTHz 3701.595091 cm-1 458.939465 meV
2 f = 22.309905 THz 140.177265 2PiTHz 744.178294 cm-1 92.266382 meV
3 f = 8.437128 THz 53.012040 2PiTHz 281.432296 cm-1 34.893170 meV
4 f = 4.421932 THz 27.783819 2PiTHz 147.499772 cm-1 18.287648 meV
5 f = 2.404480 THz 15.107791 2PiTHz 80.204807 cm-1 9.944132 meV
6 f = 1.724303 THz 10.834115 2PiTHz 57.516552 cm-1 7.131146 meV

O on Pt/GN₄-V₂C

1 f = 16.018494 THz 100.647164 2PiTHz 534.319419 cm-1 66.247189 meV
2 f = 2.715565 THz 17.062395 2PiTHz 90.581480 cm-1 11.230676 meV
3 f = 2.633697 THz 16.548008 2PiTHz 87.850684 cm-1 10.892101 meV

OOH on Pt/GN₄-V₂C

1 f = 106.371496 THz 668.351819 2PiTHz 3548.171064 cm-1 439.917303 meV
2 f = 39.893576 THz 250.658728 2PiTHz 1330.706407 cm-1 164.986626 meV
3 f = 28.634386 THz 179.915156 2PiTHz 955.140288 cm-1 118.422346 meV
4 f = 10.494069 THz 65.936178 2PiTHz 350.044443 cm-1 43.399995 meV
5 f = 4.992427 THz 31.368343 2PiTHz 166.529427 cm-1 20.647025 meV
6 f = 2.041524 THz 12.827273 2PiTHz 68.097907 cm-1 8.443067 meV
7 f = 1.823959 THz 11.460274 2PiTHz 60.840732 cm-1 7.543292 meV
8 f = 1.499895 THz 9.424121 2PiTHz 50.031124 cm-1 6.203071 meV
9 f = 0.794142 THz 4.989744 2PiTHz 26.489741 cm-1 3.284311 meV

O₂ on Pt/GN₄-V₂C

1 f = 43.241516 THz 271.694461 2PiTHz 1442.381686 cm-1 178.832601 meV
2 f = 2.437039 THz 15.312368 2PiTHz 81.290872 cm-1 10.078787 meV
3 f = 1.429444 THz 8.981458 2PiTHz 47.681101 cm-1 5.911705 meV
4 f = 1.331696 THz 8.367293 2PiTHz 44.420596 cm-1 5.507454 meV
5 f = 1.093818 THz 6.872661 2PiTHz 36.485840 cm-1 4.523669 meV
6 f = 0.546309 THz 3.432561 2PiTHz 18.222907 cm-1 2.259353 meV

OH on Rh/GN₄-V₂C

1 f = 111.012442 THz 697.511746 2PiTHz 3702.976370 cm-1 459.110722 meV
2 f = 27.763289 THz 174.441892 2PiTHz 926.083624 cm-1 114.819777 meV
3 f = 14.161583 THz 88.979851 2PiTHz 472.379551 cm-1 58.567621 meV
4 f = 5.111774 THz 32.118225 2PiTHz 170.510431 cm-1 21.140607 meV
5 f = 3.661111 THz 23.003437 2PiTHz 122.121503 cm-1 15.141142 meV
6 f = 3.118445 THz 19.593767 2PiTHz 104.020121 cm-1 12.896856 meV

O on Rh/GN₄-V_{2C}

1 f = 18.552840 THz 116.570934 2PiTHz 618.856123 cm-1 76.728408 meV
2 f = 4.561728 THz 28.662180 2PiTHz 152.162848 cm-1 18.865796 meV
3 f = 4.171288 THz 26.208977 2PiTHz 139.139197 cm-1 17.251068 meV

OOH on Rh/GN₄-V_{2C}

1 f = 108.874365 THz 684.077812 2PiTHz 3631.657803 cm-1 450.268343 meV
2 f = 38.643636 THz 242.805128 2PiTHz 1289.012918 cm-1 159.817291 meV
3 f = 24.901509 THz 156.460793 2PiTHz 830.624893 cm-1 102.984399 meV
4 f = 13.817208 THz 86.816077 2PiTHz 460.892427 cm-1 57.143399 meV
5 f = 11.492019 THz 72.206482 2PiTHz 383.332466 cm-1 47.527186 meV
6 f = 6.707036 THz 42.141553 2PiTHz 223.722648 cm-1 27.738083 meV
7 f = 3.172273 THz 19.931980 2PiTHz 105.815641 cm-1 13.119472 meV
8 f = 2.207192 THz 13.868194 2PiTHz 73.623984 cm-1 9.128214 meV
9 f = 1.824348 THz 11.462718 2PiTHz 60.853706 cm-1 7.544901 meV

O₂ on Rh/GN₄-V_{2C}

1 f = 37.101959 THz 233.118484 2PiTHz 1237.588103 cm-1 153.441424 meV
2 f = 13.650094 THz 85.766067 2PiTHz 455.318096 cm-1 56.452269 meV
3 f = 6.985620 THz 43.891947 2PiTHz 233.015205 cm-1 28.890214 meV
4 f = 3.834857 THz 24.095117 2PiTHz 127.917055 cm-1 15.859699 meV
5 f = 1.876031 THz 11.787448 2PiTHz 62.577644 cm-1 7.758642 meV
6 f = 1.713692 THz 10.767441 2PiTHz 57.162594 cm-1 7.087261 meV

OH on Ru/GN₄-V_{2C}

1 f = 110.062233 THz 691.541407 2PiTHz 3671.280812 cm-1 455.180972 meV
2 f = 26.632175 THz 167.334894 2PiTHz 888.353724 cm-1 110.141864 meV
3 f = 16.108152 THz 101.210505 2PiTHz 537.310106 cm-1 66.617987 meV
4 f = 9.223562 THz 57.953346 2PiTHz 307.664886 cm-1 38.145598 meV
5 f = 3.053211 THz 19.183892 2PiTHz 101.844161 cm-1 12.627071 meV
6 f = 2.436438 THz 15.308589 2PiTHz 81.270809 cm-1 10.076300 meV

O on Ru/GN₄-V_{2c}

1 f = 23.489402 THz 147.588265 2PiTHz 783.522083 cm-1 97.144392 meV
2 f = 4.937218 THz 31.021454 2PiTHz 164.687852 cm-1 20.418699 meV
3 f = 4.608149 THz 28.953853 2PiTHz 153.711295 cm-1 19.057779 meV

OOH on Ru/GN₄-V_{2c}

1 f = 111.106563 THz 698.103125 2PiTHz 3706.115909 cm-1 459.499975 meV
2 f = 26.013390 THz 163.446953 2PiTHz 867.713279 cm-1 107.582774 meV
3 f = 20.056649 THz 126.019639 2PiTHz 669.017762 cm-1 82.947661 meV
4 f = 10.084152 THz 63.360593 2PiTHz 336.371079 cm-1 41.704714 meV
5 f = 6.690394 THz 42.036983 2PiTHz 223.167502 cm-1 27.669254 meV
6 f = 6.285143 THz 39.490717 2PiTHz 209.649793 cm-1 25.993271 meV
7 f = 4.933245 THz 30.996495 2PiTHz 164.555348 cm-1 20.402270 meV
8 f = 2.093973 THz 13.156817 2PiTHz 69.847403 cm-1 8.659977 meV
9 f = 1.419830 THz 8.921054 2PiTHz 47.360423 cm-1 5.871946 meV

O₂ on Ru/GN₄-V_{2c}

1 f = 28.093864 THz 176.518954 2PiTHz 937.110406 cm-1 116.186924 meV
2 f = 12.490284 THz 78.478767 2PiTHz 416.631008 cm-1 51.655680 meV
3 f = 12.156114 THz 76.379116 2PiTHz 405.484297 cm-1 50.273664 meV
4 f = 5.042852 THz 31.685175 2PiTHz 168.211440 cm-1 20.855568 meV
5 f = 4.051694 THz 25.457545 2PiTHz 135.149963 cm-1 16.756466 meV
6 f = 3.386604 THz 21.278660 2PiTHz 112.964946 cm-1 14.005873 meV

4. HER Overpotential on Ni/GN_m-V_{2C} as a Function of the Nitrogen Content.

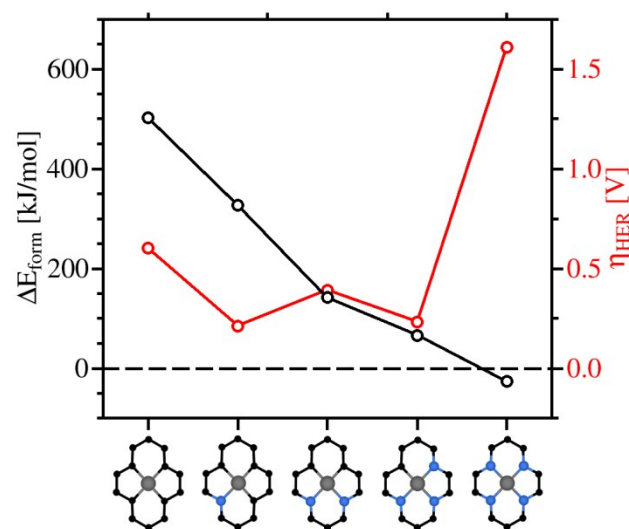


Fig. S2. Formation energies (ΔE_{form} , in kJ/mol) for Ni-decorated double vacancies in N-doped graphene and estimated HER overpotentials (η_{HER} , in V). Data points are connected to guide the eye. The corresponding structures are shown below, using the following color code: C (black), Me (gray), and N (blue).

5. HER, OER, and ORR energetics.

Table S1. Binding energies (BE) of H and O on the single-atom catalysts considered in this work,^a as well as Gibbs free reaction energies for eqs. 5, 7, 8, 9, 10, and 11 ($\Delta G_{\text{eq}\#}$) at 298 K and 1 atm. All energies are stated in kJ/mol.

	BE _H	$\Delta G_{\text{eq}5}$	BE _O	$\Delta G_{\text{eq}7}$	$\Delta G_{\text{eq}8}$	$\Delta G_{\text{eq}9}$	$\Delta G_{\text{eq}10}$	$\Delta G_{\text{eq}11}$
Ag-N ₃	-8	28	-159	113	-34	336	18	-20
Ag-N ₄	34	50	68	83	208	75	66	-19
Au-N ₃	142	169	-20	145	71	234	-17	-19
Au-N ₄	193	208	205	193	231	12	-11	-13
Co-N ₄	-3	22	15	89	156	123	22	23
Cr-N ₄	4	25	-257	-22	0	296	-9	149
Cu-N ₃	-28	7	-121	109	7	301	19	-23
Cu-N ₄	145	165	144	169	202	72	-12	-18
Fe-N ₄	3	27	-116	46	70	204	52	41
Ir-N ₄	-50	-26	-21	96	112	168	34	3
Mn-N ₄	18	42	-143	36	54	237	8	77
Mo-N ₄	-96	-78	-467	-153	-81	90 ^b	226 ^b	331
Ni-N ₃	-11	22	-60	146	31	246	16	-27
Ni-N ₄	133	155	166	183	209	58	-18	-19
Pd-N ₃	-5	28	-53	139	48	233	16	-23
Pd-N ₄	151	172	211	214	222	28	-29	-22
Pt-N ₃	44	66	-25	148	66	222	-2	-22
Pt-N ₄	115	138	181	218	190	61	-33	-23
Rh-N ₄	-37	-11	17	95	151	128	26	11
Ru-N ₄	-81	-57	-169	-1	63	211	31	108

^a $\text{BE}_X = E(X\text{-Me/GN}_m\text{-V}_{2\text{C}}) - E(\text{Me/GN}_m\text{-V}_{2\text{C}}) - \frac{1}{2} E(X_2)$;

^b OOH spontaneously dissociates on Mo/GN₄-V_{2C}, forming co-adsorbed O* and OH*.

Table S2. Magnetic moments in μ_B on metal ions and O_mH_n moieties for OER/ORR intermediates.

	*	O_2^*		OOH^*		O^*		OH^*	
	Me	Me	O ₂	Me	OOH	Me	O	Me	OH
Ag-N ₃	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.00
Ag-N ₄	0.25	0.21	-1.47	0.00	0.00	0.24	0.89	0.04	0.07
Au-N ₃	0.00	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00
Au-N ₄	0.00	0.00	1.45	0.00	0.48	0.08	0.99	0.02	0.21
Co-N ₄	0.79	0.09	0.80	0.00	0.00	0.67	0.63	0.00	0.00
Cr-N ₄	3.33	1.71	0.14	2.49	0.06	0.36	-0.03	2.51	0.06
Cu-N ₃	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.00
Cu-N ₄	0.55	0.57	1.45	0.63	0.37	0.54	0.81	0.65	0.13
Fe-N ₄	1.90	0.67	-0.55	0.96	0.12	1.22	0.58	1.09	0.11
Ir-N ₄	0.16	0.12	0.70	0.00	0.00	0.43	0.47	0.00	0.00
Mn-N ₄	3.03	2.26	0.27	2.20	0.04	0.44	0.12	2.27	0.11
Mo-N ₄	2.66	0.40	-0.01	0.44 ^a	0.05 ^a	0.36	-0.02	0.00	0.00
Ni-N ₃	0.00	0.14	1.15	0.00	0.00	0.38	0.11	0.00	0.00
Ni-N ₄	0.00	0.03	1.54	0.26	0.40	0.46	0.94	0.36	0.22
Pd-N ₃	0.00	0.01	1.54	0.00	0.00	0.00	0.00	0.00	0.00
Pd-N ₄	0.00	0.01	1.55	0.11	0.59	0.04	0.32	0.24	0.33
Pt-N ₃	0.00	0.01	1.55	0.00	0.00	0.01	0.01	0.00	0.00
Pt-N ₄	0.00	0.01	1.54	0.12	0.63	0.05	0.22	0.28	0.32
Rh-N ₄	0.17	0.07	0.79	0.00	0.00	0.37	0.54	0.00	0.00
Ru-N ₄	1.19	0.00	0.00	0.35	0.24	0.01	0.00	0.67	0.13

^a OOH spontaneously dissociates on Mo/GN₄-V_{2C}, forming co-adsorbed O* and OH*.