

Supplementary data

Theoretical insight into mercury species adsorption on graphene-based Pt Single-atom catalysts

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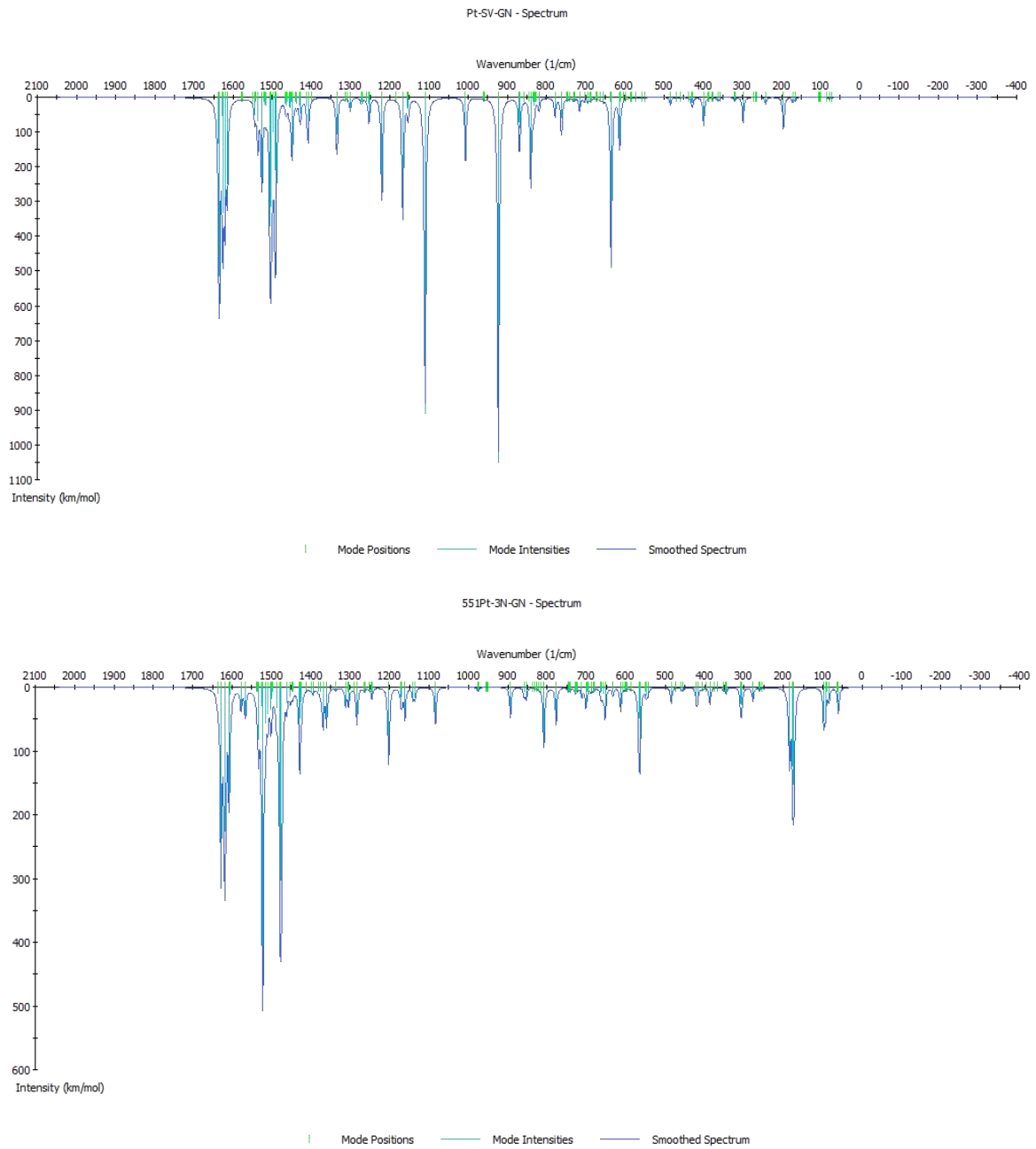


Figure S1: The IR spectrums of Pt/SV-GN and Pt/3N-GN catalysts

Table S1 The Gibbs free energy change for mercury species in Pt/SV-GN and Pt/3N-GN at a temperature range of 250-1000K

| T (K) | 1000/T (K ⁻¹) | Gibbs free energy change on Pt/SV-GN ΔG (kJ/mol) | | | | | Gibbs free energy change on Pt/3N-GN ΔG (kJ/mol) | | | | |
|--------|---------------------------|---|----------------|-------------------|----------------------------|---------------------------|---|----------------|-------------------|----------------------------|---------------------------|
| | | Hg ⁰ | HgCl molecular | HgCl dissociation | HgCl ₂ vertical | HgCl ₂ bending | Hg ⁰ | HgCl molecular | HgCl dissociation | HgCl ₂ vertical | HgCl ₂ bending |
| 250 | 4.0 | -63.910 | -220.731 | -296.043 | -102.263 | -106.496 | -99.074 | -274.238 | -357.359 | -160.419 | -314.076 |
| 275 | 3.6 | -65.740 | -222.533 | -297.264 | -104.495 | -108.473 | -99.893 | -275.070 | -357.832 | -163.061 | -315.941 |
| 298.15 | 3.4 | -67.488 | -224.246 | -298.434 | -106.606 | -110.337 | -100.675 | -275.868 | -358.292 | -165.556 | -317.709 |
| 300 | 3.3 | -67.634 | -224.388 | -298.535 | -106.781 | -110.492 | -100.737 | -275.935 | -358.333 | -165.761 | -317.855 |
| 325 | 3.1 | -69.569 | -226.286 | -299.843 | -109.114 | -112.531 | -101.611 | -276.842 | -358.873 | -168.520 | -319.824 |
| 350 | 2.9 | -71.563 | -228.234 | -301.201 | -111.501 | -114.609 | -102.497 | -277.778 | -359.445 | -171.321 | -321.834 |
| 375 | 2.7 | -73.590 | -230.215 | -302.593 | -113.925 | -116.711 | -103.408 | -278.752 | -360.051 | -174.180 | -323.904 |
| 400 | 2.5 | -75.664 | -232.238 | -304.031 | -116.391 | -118.847 | -104.336 | -279.751 | -360.683 | -177.081 | -326.010 |
| 425 | 2.4 | -77.775 | -234.299 | -305.503 | -118.899 | -121.004 | -105.281 | -280.784 | -361.343 | -180.019 | -328.155 |
| 450 | 2.2 | -79.919 | -236.389 | -306.999 | -121.432 | -123.182 | -106.242 | -281.837 | -362.029 | -183.004 | -330.341 |
| 475 | 2.1 | -82.097 | -238.513 | -308.533 | -123.999 | -125.377 | -107.220 | -282.920 | -362.743 | -186.017 | -332.560 |
| 500 | 2.0 | -84.308 | -240.670 | -310.101 | -126.603 | -127.596 | -108.211 | -284.028 | -363.483 | -189.069 | -334.818 |
| 525 | 1.9 | -86.553 | -242.860 | -311.697 | -129.232 | -129.841 | -109.219 | -285.160 | -364.248 | -192.158 | -337.108 |
| 550 | 1.8 | -88.822 | -245.079 | -313.323 | -131.895 | -132.102 | -110.238 | -286.314 | -365.038 | -195.280 | -339.432 |
| 575 | 1.7 | -91.121 | -247.320 | -314.974 | -134.583 | -134.380 | -111.271 | -287.493 | -365.845 | -198.432 | -341.786 |
| 600 | 1.7 | -93.441 | -249.581 | -316.642 | -137.291 | -136.671 | -112.320 | -288.692 | -366.677 | -201.617 | -344.172 |
| 625 | 1.6 | -95.790 | -251.876 | -318.348 | -140.029 | -138.983 | -113.373 | -289.909 | -367.529 | -204.827 | -346.580 |
| 650 | 1.5 | -98.165 | -254.188 | -320.070 | -142.792 | -141.311 | -114.444 | -291.146 | -368.399 | -208.071 | -349.030 |
| 675 | 1.5 | -100.560 | -256.528 | -321.817 | -145.576 | -143.652 | -115.526 | -292.404 | -369.293 | -211.336 | -351.496 |
| 700 | 1.4 | -102.980 | -258.886 | -323.589 | -148.381 | -146.009 | -116.621 | -293.679 | -370.205 | -214.630 | -353.991 |

| T (K) | 1000/T (K ⁻¹) | Gibbs free energy change on Pt/SV-GN ΔG (kJ/mol) | | | | | Gibbs free energy change on Pt/3N-GN ΔG (kJ/mol) | | | | |
|-------|---------------------------|---|-------------------|----------------------|-------------------------------|------------------------------|---|-------------------|----------------------|-------------------------------|------------------------------|
| | | Hg ⁰ | HgCl molecular | HgCl dissociation | HgCl ₂ vertical | HgCl ₂ bending | Hg ⁰ | HgCl molecular | HgCl dissociation | HgCl ₂ vertical | HgCl ₂ bending |
| 725 | 1.4 | -105.417 | -261.269 | -325.379 | -151.202 | -148.375 | -117.721 | -294.971 | -371.128 | -217.944 | -356.508 |
| 750 | 1.3 | -107.875 | -263.668 | -327.188 | -154.049 | -150.762 | -118.837 | -296.287 | -372.081 | -221.288 | -359.053 |
| 775 | 1.3 | -110.358 | -266.092 | -329.023 | -156.921 | -153.161 | -119.957 | -297.617 | -373.043 | -224.657 | -361.620 |
| 800 | 1.3 | -112.857 | -268.533 | -330.871 | -159.805 | -155.569 | -121.094 | -298.963 | -374.025 | -228.052 | -364.215 |
| 825 | 1.2 | -115.374 | -270.995 | -332.744 | -162.710 | -157.993 | -122.239 | -300.330 | -375.028 | -231.462 | -366.832 |
| 850 | 1.2 | -117.911 | -273.470 | -334.633 | -165.632 | -160.426 | -123.393 | -301.705 | -376.044 | -234.898 | -369.466 |
| 875 | 1.1 | -120.469 | -275.970 | -336.539 | -168.570 | -162.871 | -124.559 | -303.101 | -377.077 | -238.355 | -372.124 |
| 900 | 1.1 | -123.040 | -278.482 | -338.462 | -171.525 | -165.329 | -125.734 | -304.510 | -378.122 | -241.837 | -374.808 |
| 925 | 1.1 | -125.627 | -281.011 | -340.401 | -174.502 | -167.804 | -126.912 | -305.931 | -379.179 | -245.336 | -377.508 |
| 950 | 1.1 | -128.236 | -283.561 | -342.362 | -177.494 | -170.282 | -128.108 | -307.373 | -380.262 | -248.855 | -380.229 |
| 975 | 1.0 | -130.852 | -286.119 | -344.331 | -180.496 | -172.769 | -129.308 | -308.827 | -381.353 | -252.396 | -382.967 |
| 1000 | 1.0 | -133.490 | -288.698 | -346.320 | -183.518 | -175.269 | -130.520 | -310.299 | -382.460 | -255.957 | -385.730 |