**Supporting information**

New Progress on Surface specific interactions and Lewis’s acid-base properties of solid surfaces

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**Table S1.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on silica particles at different temperatures.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Temperature T (K) | 323.15 | 343.15 | 363.15 | 383.15 | 403.15 |
| C5 | 19.780 | 19.780 | 18.187 | 16.600 | 15.444 |
| C6 | 23.409 | 23.409 | 21.524 | 19.646 | 18.277 |
| C7 | 26.534 | 26.534 | 24.397 | 22.269 | 20.718 |
| C8 | 30.814 | 30.814 | 28.333 | 25.861 | 24.060 |
| C9 | 33.503 | 33.503 | 30.805 | 28.117 | 26.159 |
| CCl4 | 24.557 | 22.516 | 20.703 | 18.896 | 17.580 |
| Nitromethane | 16.440 | 15.074 | 13.860 | 12.651 | 11.770 |
| CH2Cl2 | 16.229 | 14.880 | 13.682 | 12.488 | 11.618 |
| CHCl3 | 19.992 | 18.330 | 16.854 | 15.383 | 14.312 |
| Diethyl ether | 19.744 | 18.102 | 16.645 | 15.192 | 14.134 |
| THF | 17.029 | 15.613 | 14.356 | 13.103 | 12.191 |
| Ethyl Acetate | 19.548 | 17.923 | 16.480 | 15.042 | 13.994 |
| Acetone | 13.404 | 12.289 | 11.300 | 10.314 | 9.595 |
| Acetonitrile | 10.305 | 9.449 | 8.688 | 7.930 | 7.377 |
| Toluene  | 23.754 | 21.779 | 20.025 | 18.278 | 17.005 |
| Benzene | 21.295 | 19.525 | 17.953 | 16.386 | 15.245 |

**Table S2.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on silica particles at different temperatures.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Temprature T(K)** | **323.15** | **343.15** | **363.15** | **383.15** | **403.15** |
| CCl4 | 6.752 | 6.810 | 6.881 | 6.968 | 7.129 |
| Nitromethane | 13.573 | 12.367 | 11.273 | 10.191 | 9.378 |
| CH2Cl2 | 22.490 | 21.846 | 21.269 | 20.716 | 20.287 |
| CHCl3 | 19.752 | 19.304 | 18.925 | 18.546 | 18.250 |
| Diethyl ether | 26.838 | 25.462 | 23.802 | 22.314 | 20.676 |
| THF | 35.506 | 32.787 | 30.435 | 27.908 | 25.593 |
| Ethyl Acetate | 4.566 | 4.015 | 3.530 | 3.079 | 2.732 |
| Acetone | 10.612 | 9.608 | 8.703 | 7.816 | 7.144 |
| Acetonitrile | 16.734 | 15.304 | 14.016 | 12.738 | 11.793 |
| Toluene  | 17.330 | 16.724 | 16.168 | 15.598 | 15.187 |
| Benzene | 5.640 | 5.170 | 4.745 | 4.328 | 4.026 |

**Table S3.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on MgO particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Temperature (K) | 323.15 | 343.15 | 363.15 | 383.15 |
| C6 | 19.996 | 19.127 | 18.299 | 17.531 |
| C7 | 22.673 | 21.688 | 20.748 | 19.877 |
| C8 | 26.336 | 25.192 | 24.100 | 23.089 |
| C9 | 28.638 | 27.394 | 26.207 | 25.107 |
| CH2Cl2 | 12.689 | 12.138 | 11.612 | 11.125 |
| CHCl3 | 15.630 | 14.951 | 14.303 | 13.703 |
| Diethyl ether | 15.479 | 14.806 | 14.165 | 13.570 |
| THF | 13.353 | 12.773 | 12.220 | 11.707 |
| Ethyl Acetate | 15.313 | 14.648 | 14.013 | 13.425 |
| Acetone | 10.505 | 10.048 | 9.613 | 9.210 |
| Acetonitrile | 8.048 | 7.699 | 7.365 | 7.056 |
| Toluene  | 18.645 | 17.835 | 17.062 | 16.346 |

**Table S4.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on MgO particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | **323.15** | **343.15** | **363.15** | **383.15** |
| CH2Cl2 | 3.312 | 3.786 | 4.532 | 5.211 |
| CHCl3 | 5.833 | 2.693 | 1.560 | 2.176 |
| Diethyl ether | 14.415 | 16.559 | 18.671 | 20.721 |
| THF | 23.053 | 25.004 | 26.928 | 28.797 |
| Ethyl Acetate | 6.224 | 7.620 | 9.112 | 10.523 |
| Acetone | 15.723 | 20.520 | 25.354 | 30.243 |
| Acetonitrile | 24.370 | 26.000 | 27.633 | 29.269 |
| Toluene  | 10.771 | 10.471 | 10.192 | 9.945 |

**Table S5.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on ZnO particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **T(K)** | 323.15 | 343.15 | 363.15 | 383.15 |
| C6 | 12.6777 | 11.3464 | 10.2409 | 9.2860 |
| C7 | 14.4122 | 12.8988 | 11.6421 | 10.5565 |
| C8 | 16.7694 | 15.0085 | 13.5462 | 12.2831 |
| C9 | 18.2572 | 16.3401 | 14.7481 | 13.3728 |
| DCM | 7.9317 | 7.0988 | 6.4071 | 5.8097 |
| TCM | 9.7642 | 8.7389 | 7.8875 | 7.1520 |
| Diethyl ether | 9.8951 | 8.8560 | 7.9932 | 7.2478 |
| THF | 8.5518 | 7.6537 | 6.9080 | 6.2639 |
| Ethyl Acetate | 9.7236 | 8.7025 | 7.8546 | 7.1222 |
| Benzene | 10.7177 | 9.5922 | 8.6577 | 7.8504 |

**Table S6.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on ZnO particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | **323.15** | **343.15** | **363.15** | **383.15** |
| DCM | 2.449 | 1.915 | 1.223 | 0.632 |
| TCM | 1.151 | 1.061 | 0.999 | 0.933 |
| Diethyl ether | 7.721 | 7.045 | 6.594 | 6.037 |
| THF | 13.596 | 12.901 | 12.294 | 11.517 |
| Ethyl Acetate | 3.955 | 2.715 | 1.800 | 1.042 |
| Benzene | 0.870 | 0.690 | 0.537 | 0.354 |

**Table S7.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on monogal-Zn particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T (K) | 323.15 | 343.15 | 363.15 | 383.15 |
| C6 | 25.249 | 23.667 | 21.355 | 18.899 |
| C7 | 28.600 | 26.809 | 24.189 | 21.408 |
| C8 | 33.199 | 31.119 | 28.078 | 24.850 |
| C9 | 36.084 | 33.823 | 30.518 | 27.009 |
| DCM | 16.113 | 15.103 | 13.628 | 12.061 |
| TCM | 16.610 | 15.570 | 14.048 | 12.433 |
| Diethyl ether | 15.260 | 14.304 | 12.906 | 11.422 |
| THF | 15.156 | 14.206 | 12.818 | 11.344 |
| Ethyl Acetate | 19.324 | 18.114 | 16.344 | 14.464 |
| Acetone | 15.412 | 14.447 | 13.035 | 11.536 |
| Acetonitrile | 17.138 | 16.064 | 14.494 | 12.828 |
| Toluene  | 14.696 | 13.775 | 12.429 | 11.000 |

**Table S8.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on monogal-Zn particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | **323.15** | **343.15** | **363.15** | **383.15** |
| DCM | 2.354 | 1.965 | 1.426 | 0.854 |
| TCM | 15.001 | 11.698 | 7.938 | 6.927 |
| Diethyl ether | 17.481 | 15.950 | 14.408 | 12.982 |
| THF | 23.786 | 21.503 | 19.298 | 17.285 |
| Ethyl Acetate | 12.287 | 9.154 | 5.642 | 4.895 |
| Acetone | 22.779 | 20.603 | 18.500 | 16.582 |
| Acetonitrile | 19.104 | 16.905 | 14.694 | 12.454 |
| Toluene  | 22.246 | 20.175 | 18.138 | 16.267 |

**Table S9.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on alumina particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T (K) | 323.15 | 343.15 | 363.15 | 383.15 |
| C6 | 21.488 | 20.220 | 19.103 | 18.422 |
| C7 | 24.393 | 22.954 | 21.685 | 20.912 |
| C8 | 28.356 | 26.682 | 25.208 | 24.310 |
| C9 | 30.852 | 29.030 | 27.427 | 26.449 |
| CCl4 | 20.481 | 19.272 | 18.207 | 17.559 |
| CH2Cl2 | 13.549 | 12.749 | 12.044 | 11.615 |
| CHCl3 | 16.684 | 15.699 | 14.832 | 14.303 |
| Ether | 16.696 | 15.710 | 14.842 | 14.313 |
| THF | 14.415 | 13.564 | 12.815 | 12.358 |
| Ethyl acetate | 16.467 | 15.495 | 14.639 | 14.117 |
| Toluene | 20.200 | 19.008 | 17.958 | 17.318 |

**Table S10.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on alumina particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | **323.15** | **343.15** | **363.15** | **383.15** |
| CCl4 | 6.751 | 6.654 | 6.575 | 6.648 |
| CH2Cl2 | 38.808 | 36.648 | 34.670 | 32.613 |
| CHCl3 | 18.559 | 16.226 | 14.028 | 12.322 |
| Ether | 41.085 | 39.144 | 37.268 | 35.790 |
| THF | 40.532 | 38.377 | 36.371 | 34.878 |
| Ethyl acetate | 11.624 | 9.452 | 7.875 | 6.125 |
| Toluene | 18.821 | 17.490 | 16.418 | 15.980 |

**Table S11.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on TiO2 particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T (K) | **313.15** | **333.15** | **353.15** | **373.15** |
| C6 | 21.431 | 21.007 | 20.582 | 20.165 |
| C7 | 24.274 | 23.793 | 23.313 | 22.841 |
| C8 | 28.176 | 27.618 | 27.060 | 26.512 |
| C9 | 30.623 | 30.017 | 29.410 | 28.815 |
| CH2Cl2 | 13.681 | 13.410 | 13.139 | 12.873 |
| CHCl3 | 16.855 | 16.521 | 16.187 | 15.859 |
| THF | 14.252 | 13.970 | 13.688 | 13.410 |
| Ethyl Acetate | 16.401 | 16.077 | 15.752 | 15.433 |
| Acetone | 11.233 | 11.010 | 10.788 | 10.569 |
| Benzene | 17.813 | 17.460 | 17.108 | 16.761 |
| Nitromethane | 13.847 | 13.573 | 13.299 | 13.030 |
| Acetonitrile | 8.711 | 8.539 | 8.366 | 8.197 |

**Table S12.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on TiO2 particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | **313.15** | **333.15** | **353.15** | **373.15** |
| CH2Cl2 | 2.546 | 1.924 | 1.254 | 0.723 |
| CHCl3 | 3.146 | 2.019 | 0.893 |   |
| THF | 7.620 | 6.620 | 5.620 | 4.620 |
| Ethyl Acetate | 3.979 | 2.417 | 0.857 | -0.710 |
| Acetone | 5.776 | 4.068 | 2.362 | 0.651 |
| Benzene | 5.564 | 4.199 | 2.834 | 1.463 |
| Nitromethane | 10.394 | 9.024 | 7.657 | 6.283 |
| Acetonitrile | 4.615 | 2.524 | 0.433 |   |

**Table S13.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on untreated carbon fibers particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T (K) | **313.15** | **333.15** | **353.15** | **373.15** |
| C6 | 20.723 | 19.965 | 19.206 | 18.959 |
| C7 | 23.452 | 22.594 | 21.736 | 21.456 |
| C8 | 27.206 | 26.211 | 25.215 | 24.891 |
| C9 | 29.558 | 28.476 | 27.395 | 27.042 |
| CCl4 | 20.133 | 19.396 | 18.659 | 18.419 |
| CH2Cl2 | 13.291 | 12.805 | 12.318 | 12.160 |
| CHCl3 | 16.378 | 15.779 | 15.179 | 14.984 |
| Ether | 15.944 | 15.361 | 14.777 | 14.587 |
| THF | 13.736 | 13.234 | 12.731 | 12.567 |
| C6H6 | 17.158 | 16.530 | 15.902 | 15.697 |
| Ethyl acetate | 15.851 | 15.271 | 14.691 | 14.502 |
| Acetone | 10.842 | 10.445 | 10.048 | 9.919 |

**Table S14.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on untreated carbon fibers particles at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | 313.15 | 333.15 | 353.15 | 373.15 |
| CCl4 | 1.723 | 1.956 | 2.203 | 2.518 |
| CH2Cl2 | 4.096 | 3.645 | 3.129 | 2.548 |
| CHCl3 | 14.829 | 13.537 | 11.761 | 8.193 |
| Ether | 2.112 | 1.633 | 1.131 | 0.546 |
| THF | 11.852 | 11.079 | 10.310 | 9.748 |
| C6H6 | 8.577 | 8.315 | 8.055 | 8.011 |
| Ethyl acetate | 9.500 | 9.251 | 9.019 | 8.975 |
| Acetone | 10.723 | 10.282 | 9.865 | 9.647 |

**Table S15.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{d}\left(T\right)$) of n-alkanes and polar solvents adsorbed on oxidized carbon fibers at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T (K) | **313.15** | **333.15** | **353.15** | **373.15** |
| C6 | 20.674 | 19.429 | 18.209 | 16.997 |
| C7 | 23.396 | 21.988 | 20.607 | 19.236 |
| C8 | 27.142 | 25.507 | 23.906 | 22.315 |
| C9 | 29.488 | 27.712 | 25.972 | 24.244 |
| CCl4 | 20.085 | 18.875 | 17.690 | 16.513 |
| CH2Cl2 | 13.260 | 12.461 | 11.679 | 10.902 |
| CHCl3 | 16.339 | 15.355 | 14.391 | 13.433 |
| Ether | 15.906 | 14.948 | 14.010 | 13.077 |
| THF | 13.704 | 12.879 | 12.070 | 11.267 |
| C6H6 | 17.117 | 16.086 | 15.076 | 14.073 |
| Ethyl acetate | 15.814 | 14.862 | 13.928 | 13.001 |
| Acetone | 10.816 | 10.165 | 9.526 | 8.892 |

**Table S16.** Values (in kJ/mol) of London dispersive energy ($-∆G\_{a}^{sp}\left(T\right)$) of polar solvents adsorbed on oxidized carbon fibers at different temperatures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | 313.15 | 333.15 | 353.15 | 373.15 |
| CCl4 | 2.785 | 2.843 | 2.911 | 2.974 |
| CH2Cl2 | 10.546 | 9.952 | 9.379 | 8.800 |
| CHCl3 | 12.788 | 12.228 | 11.685 | 11.134 |
| Ether | 7.399 | 6.965 | 6.548 | 6.124 |
| THF | 17.020 | 15.878 | 14.753 | 13.623 |
| C6H6 | 10.429 | 9.943 | 9.473 | 8.995 |
| Ethyl acetate | 13.212 | 12.718 | 12.242 | 11.758 |
| Acetone | 17.928 | 16.999 | 16.094 | 15.183 |