Supporting information

N, S Co-Doped Porous Carbon for Ultra-Selective and Cost-Effective Capture of Palladium from Highly Acidic Solution

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Text S1. Data reduction, data analysis, and EXAFS fitting

Data reduction, data analysis, and EXAFS fitting were performed and analyzed with the Athena and Artemis programs of the Demeter data analysis packages[1] that utilizes the FEFF6 program[2] to fit the EXAFS data. The energy calibration of the sample was conducted through standard and Pd foil, which as a reference was simultaneously measured. A linear function was subtracted from the pre-edge region, then the edge jump was normalized using Athena software. The χ(k) data was isolated by subtracting a smooth, third-order polynomial approximating the absorption background of an isolated atom. The k^3-weighted χ(k) data were Fourier transformed after applying a HanFeng window function (Δk = 1.0). For EXAFS modeling, The global amplitude EXAFS (CN, R, σ^2 and ΔE_0) were obtained by nonlinear fitting, with least-squares refinement, of the EXAFS equation to the Fourier-transformed data in R-space, using Artemis software, EXAFS of the Pd foil are fitted and the obtained amplitude reduction factor S_0^2 value (0.809) was set in the EXAFS analysis to determine the coordination numbers (CNs) in sample.

Text S2. Computational methodology

Density functional theory (DFT) calculations were carried out using the Gaussian 16 A.03 program package.[3] Geometry optimizations and harmonic frequency calculations were carried out in highly-polarized implicit aqueous (ε = 78.36) by solvation model based on density (SMD)[4] at the level of B3LYP[5-7]-D3(BJ)[8]/Def2-SVP[9, 10]. Single point energy refinements were performed on the optimized structures in the same solvent at the level of M06[11]-D3[12]/Def2-TZVP. The atomic charges conducted by natural population analysis (NPA)[13] were utilized. All thermodynamic

data were reported in 298.15 K and 1 atm. All DFT-optimized configurations of SPC, NPC, and NSPC sorbents and after Pd(II) adsorption are listed in following:

NPC

-2 1

C 2.75662 -5.49185 -0.89216
C 4.85741 -4.76065 0.15949
C 4.07754 -5.75845 -0.4651
C 6.7966 -3.6339 1.27921
C 6.14819 -4.79298 0.72637
C -1.49814 -2.97267 -0.36929
C -2.17264 -4.14791 -0.83315
C -0.00373 -5.23327 -1.32711
C 0.7127 -4.15395 -0.83347
C 2.9196 -3.17396 -0.27059
C 4.19924 -3.52131 0.1618
C 4.79587 -2.35532 0.61757
C 4.34653 0.03708 0.6373
C 3.86392 -1.29124 0.38828
C 6.35257 1.41251 1.2821
C 8.27224 0.39612 2.48116
C 7.59032 1.59506 2.06226
C -3.48965 -1.98265 0.25662
C -3.30879 0.32719 1.21589
C -4.11921 -0.85966 0.78216
C 0.22977 2.66747 -0.20596
C 1.67342 2.455 -0.22523
C 3.63402 1.27529 0.32066
C 4.45224 2.44294 0.11525
C 4.69006 4.68776 -0.91996
C 3.86814 3.57044 -0.52791
C 5.80488 2.50301 0.55712
C 6.59425 3.63978 0.17535
C 6.07395 4.65583 -0.57087
C -5.42403 1.57179 1.18097
C -5.52985 3.99604 0.77357
C -4.0297 1.59568 0.90046
C -3.37583 2.75032 0.47094
C -4.17732 3.979 0.29518
C -1.95958 2.83768 0.13822
C -1.56455 4.03551 -0.51478
C -2.28595 5.20693 -0.8083
C -0.20598 3.90844 -0.74326
C 0.52463 4.95218 -1.28339
C -0.14665 6.13995 -1.68062
C 7.76913 -0.83607 2.19565
C -1.56469 6.24648 -1.44648
C 6.51274 -1.02331 1.53457
C -6.12025 0.33254 1.34645
C -4.26014 -3.12983 -0.10123
C -3.57981 -4.21079 -0.69536
C -6.24176 -2.04299 0.80437
C -5.65256 -3.17455 0.17998
C -4.31237 -5.37077 -1.10716
C -2.17797 -6.37209 -1.82407
C -6.43265 -4.38827 -0.21399
C 0.6773 -6.42976 -1.76078
C 2.02642 -6.52431 -1.52009
C -5.69888 -5.40931 -0.87365
C -3.57109 -6.41685 -1.71024
C -7.58812 -2.04134 1.27279
C -7.47317 0.31941 1.73835
H -8.11292 -2.98716 1.1779
C -8.175 -0.91725 1.77028
H 7.63992 3.6659 0.4639
H 8.30496 -1.74209 2.47094
C 5.70978 0.1331 1.16754
N -0.87265 2.0049 0.31904
N -2.12594 -1.94074 0.1152
N -5.48301 -0.87547 0.99346
N 2.69369 -1.81801 -0.14682
N 2.28756 1.32257 0.18934
C 2.46801 3.59189 -0.72027
C -1.4513 -5.23148 -1.3525
C 6.06736 -2.31758 1.17965
C -6.16103 2.78043 1.25602
C -3.66625 5.19237 -0.31557
C 0.01858 -2.87763 -0.38367
H -2.34836 0.28332 0.70274
H 0.27813 -2.0918 -1.11998
O 0.42957 -2.47223 0.9045
H 1.24756 -1.93449 0.72339
O -2.97541 0.23081 2.61129
H -3.77633 0.39637 3.13239
O 4.54508 -7.02456 -0.67722
H 5.50119 -7.04131 -0.51577
O 7.94184 -3.72222 1.81129
O 8.04395 2.72715 2.37372

O -7.67835 -4.5107 0.00019
C 1.9259 4.79133 -1.28035
N 2.09944 -4.22188 -0.69729
C -8.12414 1.55138 2.00211
C -7.49671 2.74417 1.73655
C -1.43591 -7.49002 -2.37
C -0.07861 -7.51594 -2.33581
C 2.71575 5.87873 -1.73777
C 0.68277 7.17818 -2.21737
C 2.05321 7.04425 -2.24723
C 4.11841 5.79542 -1.58088
O 4.84577 6.83907 -2.0298
H 5.79609 6.68813 -1.912
C -6.29019 5.18818 0.70639
C -4.47722 6.33145 -0.38014
H -4.08159 7.23292 -0.83687
C -5.77205 6.33676 0.14339
O -2.21655 7.38889 -1.80264
H -6.37671 7.24475 0.09231
H -7.31226 5.20232 1.07882
H -8.05207 3.66809 1.88567
H -9.15666 1.52927 2.35463
H -9.20439 -0.9356 2.13284
H -6.27008 -6.28744 -1.18507
H -4.09894 -7.3067 -2.06202
H -1.99965 -8.33236 -2.77722
H 0.47533 -8.38016 -2.70932
H 2.56215 -7.44037 -1.76162
H 6.72024 -5.7226 0.78331
H 9.21143 0.52324 3.02541
H 6.74003 5.46874 -0.86958
H 2.6634 7.86129 -2.63303
H 0.24926 8.11058 -2.5884
H -1.60029 8.02674 -2.19217

NSPC

-2 1

C 0.7505 -5.57845 -1.28004
C 3.0477 -5.6109 -0.43894
C 1.9615 -6.26783 -1.05342
C 5.25982 -5.21713 0.56845
C 4.32684 -6.07966 -0.00932
C -2.42547 -1.9527 -0.02291
C -3.4864 -2.83779 -0.42234
C -1.83904 -4.50076 -1.2313
C -0.77525 -3.73591 -0.78515
C 1.66687 -3.46865 -0.51008
C 2.82397 -4.24755 -0.26444
C 3.76851 -3.38616 0.25427
C 4.04043 -1.0286 0.61349
C 3.19322 -2.07229 0.22117
C 6.24383 -0.32401 1.5051
C 7.68183 -1.94997 2.64722
C 7.39727 -0.56524 2.3437
C -3.93441 -0.28385 0.53331
C -2.97467 1.95917 1.13301
C -4.14282 1.04737 0.88493
C 3.60952 0.42775 0.67054
C 4.76707 1.3689 0.3848
C 5.78877 3.37128 -0.67074
C 4.59194 2.61224 -0.30122
C 6.03061 0.97925 0.87467
C 7.15856 1.79971 0.59798
C 7.04105 2.91971 -0.18221
C -4.57874 3.80645 0.86145
C -3.91947 6.03847 0.14171
C -3.27535 3.34379 0.66553
C -2.26562 4.1959 0.14607
C -2.63719 5.55348 -0.18651
C -0.0772 4.50265 -0.59808
C -0.39833 5.87191 -1.09193
C 1.29119 4.08346 -0.7388
C 2.14257 5.01058 -1.38895
C 1.86463 6.29773 -1.91993
C 6.94192 -2.98383 2.14052
C 0.55155 6.72105 -1.76904
C 5.77804 -2.75538 1.35073
C -5.64546 2.90385 1.18913
C -5.06096 -1.14553 0.34171
C -4.81841 -2.42569 -0.19464
C -6.53511 0.63937 1.0997
C -6.36972 -0.70684 0.67052
C -5.91949 -3.28514 -0.50589
C -4.30636 -4.89248 -1.43079

C -7.52041 -1.64277 0.48195
C -1.6186 -5.78927 -1.84761
C -0.3361 -6.28479 -1.84347
C -7.2169 -2.87164 -0.16165
C -5.61865 -4.50816 -1.15648
C -7.78891 1.15796 1.51646
C -6.92386 3.40518 1.49354
H -8.58999 0.42913 1.59411
C -7.97884 2.49354 1.73753
H 8.12857 1.50554 0.98766
H 7.21924 -4.00174 2.42005
C 5.34191 -1.38216 1.1585
N -2.63894 -0.73027 0.38239
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C -1.01748 -2.49312 0.02071
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H -0.28453 -1.71064 -0.20507
O -2.59255 1.93274 2.51674
H -3.25999 2.4177 3.02682
O 2.00514 -7.58526 -1.42223
H 2.93018 -7.87183 -1.47375
O 6.45269 -5.77887 0.9187
O 8.15128 0.34767 2.8208
O -8.70842 -1.36418 0.8308
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N 0.54125 -4.19909 -0.90253
C -7.16069 4.82186 1.46797
C -6.19836 5.68383 1.03569
C -4.01877 -6.1418 -2.12484
C -2.73547 -6.55437 -2.32926
C 4.55696 5.19068 -1.76319
C 3.01886 6.99359 -2.46955
C 4.29016 6.46912 -2.39482
C 5.76773 4.59322 -1.44291
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O 0.07934 7.94419 -2.18639
H -6.40188 6.75319 0.94606
H -8.15632 5.17513 1.74227
H -8.95574 2.87545 2.03983
H -8.06407 -3.52852 -0.37371
H -6.43771 -5.16536 -1.44899
H -2.54296 -7.50939 -2.82419
H -0.13819 -7.29035 -2.20938
H 4.61779 -7.12486 -0.13131
H 8.54569 -2.14165 3.28966
H 7.9488 3.49036 -0.39076
H 5.12637 7.0455 -2.79718
H 2.88723 7.9735 -2.93684
H 0.80626 8.46244 -2.56158
N -1.01033 3.73063 -0.03387
N 2.01127 2.99191 -0.28068
H 2.80011 0.60404 -0.04571
O -5.10558 -6.84657 -2.5229
H -4.82439 -7.66885 -2.95577
H -1.94371 7.36927 -1.12144
H -4.15333 7.0897 -0.04386
H 7.12316 -5.09034 1.04222
S -0.61672 -2.88933 1.81751
H -1.66727 -3.73043 1.98622
O 3.00242 0.71304 1.95384
H 3.69219 0.59071 2.62404

SPC

0 1

C -0.67308 -5.43084 1.52841
C -2.99062 -4.99701 2.08586
C -1.87184 -5.81013 2.2107
C -5.42251 -4.54754 2.14784
C -4.33613 -5.32429 2.47523
C 2.18195 -2.54067 -1.22981
C 3.18839 -3.56661 -1.23538
C 1.60653 -5.04709 -0.07417
C 0.63421 -4.02501 0.01105
C -1.58855 -3.17324 0.96899
C -2.77057 -3.73083 1.48607
C -3.90338 -2.9127 1.25346
C -4.44102 -0.88585 0.12673

C -3.49139 -1.71313 0.72227
C -6.75422 -0.47645 -0.6258
C -8.49541 -2.19513 -0.11413
C -8.1548 -0.95149 -0.77953
C 3.93927 -0.88352 -1.29145
C 3.17448 1.29401 -0.42666
C 4.28964 0.3637 -0.78573
C -1.04049 2.5056 -0.195
C -2.29097 2.02534 -0.54529
C -3.98534 0.32199 -0.43126
C -4.95123 1.21385 -0.9723
C -5.56777 3.52647 -1.68429
C -4.59355 2.5777 -1.25197
C -6.32002 0.79468 -1.12239
C -7.22633 1.73545 -1.72552
C -6.8732 3.03044 -1.98581
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C 4.16611 4.67267 2.05921
C 3.53464 2.35675 0.56216
C 2.46431 3.17701 1.00888
C 2.82864 4.47472 1.59476
C 1.08082 2.92672 0.71794
C 0.34592 4.14733 0.57655
C 0.67378 5.46922 0.94759
C -0.85301 3.89125 -0.06939
C -1.77344 4.85302 -0.39995
C -1.46453 6.21796 -0.11801
C -7.59826 -2.92529 0.59678
C -0.24071 6.50466 0.56178
C -6.22707 -2.5178 0.73298
C 5.93927 1.81342 0.28532
C 4.94951 -1.87796 -1.49512
C 4.53714 -3.23963 -1.51999
C 6.67844 -0.23258 -0.94367
C 6.32896 -1.51905 -1.47052
C 5.5337 -4.27407 -1.59311
C 3.842 -5.89046 -0.83988
C 7.33414 -2.55822 -1.83425
C 1.42635 -6.28809 0.61413
C 0.29642 -6.44312 1.39747
C 6.87113 -3.90423 -1.83535
C 5.12629 -5.60324 -1.3167
C 8.0342 0.16541 -0.68671
C 7.28588 2.1028 0.59543
H 8.82482 -0.47637 -1.06473
C 8.3223 1.27897 0.05582
H -8.23636 1.4004 -1.92995
H -7.9199 -3.8748 1.01933
C -5.8226 -1.29637 0.08268
C -3.28281 2.99493 -0.94794
C 2.85009 -4.85899 -0.79083
C -5.25181 -3.31605 1.39177
C 5.21759 3.74487 1.68137
C 1.92509 5.59055 1.66582
C 0.75432 -2.90044 -0.97254
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H 0.20747 -2.01167 -0.64948
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H 3.30957 2.3559 -2.07048
O -1.88195 -7.00244 2.84448
H -2.75091 -7.17701 3.23828
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C 2.38499 -7.35623 0.44946
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C -3.64639 6.75812 -1.09231
C -5.24833 4.91421 -1.71881
O -6.13821 5.85386 -2.0926
H -7.00208 5.46564 -2.29976
C 4.4783 5.83799 2.79175
C 2.29426 6.74874 2.37652
H 1.58919 7.57178 2.44937
C 3.54303 6.84642 2.98073
O 0.092 7.7807 0.87002
H 3.80498 7.7346 3.55833
H 5.47675 5.9693 3.20395
H 6.85963 4.7919 2.6572
H 8.61812 3.38837 1.71837
H 9.35975 1.54071 0.27651
H 7.63042 -4.68025 -1.96563

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H 4.2556 -7.98719 -0.36715
H 2.17147 -8.311 0.9361
H 0.12366 -7.39807 1.89167
H -4.54467 -6.2428 3.02786
H -9.52591 -2.53428 -0.23843
H -7.63594 3.69239 -2.40319
H -4.38317 7.50772 -1.383
H -2.30267 8.24264 -0.38495
H -0.58147 8.40263 0.55536
S -0.15153 -3.33464 -2.5671
H 0.61361 -4.41307 -2.86009
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C 2.55413 -1.24241 -1.3618
C -2.57094 0.65362 -0.30019
C -1.98642 -1.56641 0.82587
C -0.50683 -4.12987 0.85486
C 0.05567 1.781 0.32482
H 1.78908 -0.47096 -1.39053
C -1.51536 -0.19175 0.21811
C -0.21984 0.39412 0.51194
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H -1.82712 -1.34166 1.90105
H -7.2416 -4.24885 2.72931

NPC-Pd^{II}

0 1

C 2.3105 -5.30421 -1.50886
C 4.55465 -4.73415 -0.68374
C 3.68723 -5.60603 -1.38255
C 6.64112 -3.86862 0.40804
C 5.89844 -4.88255 -0.29819
C -1.7398 -2.93442 0.05055
C -2.50761 -4.05716 -0.39141
C -0.48256 -5.08189 -1.34003
C 0.327 -4.05998 -0.84896
C 2.59338 -3.12934 -0.52428
C 3.91772 -3.52518 -0.35639
C 4.60147 -2.4946 0.27747
C 4.2552 -0.16396 0.79593
C 3.70631 -1.41322 0.40529
C 6.25374 1.01655 1.71819
C 8.21256 -0.27828 2.55304
C 7.50118 0.98225 2.5148
C -3.62236 -1.81917 0.74081
C -3.31339 0.60837 1.25967
C -4.18433 -0.60462 1.10793
C 0.33806 2.59914 -0.38346
C 1.74605 2.38412 -0.18929
C 3.60955 1.10168 0.57147
C 4.42506 2.27543 0.63903
C 4.79719 4.6279 -0.06176
C 3.94648 3.47711 0.03931
C 5.72393 2.24174 1.24287
C 6.50696 3.44734 1.21344
C 6.08322 4.56384 0.55744
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C -5.42707 4.15611 0.02429
C -3.99753 1.8037 0.68104
C -3.30151 2.81866 0.02231
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C -1.38429 3.93882 -0.98852
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C -0.00794 3.81324 -1.02065
C 0.81263 4.87402 -1.3689
C 0.22379 6.07678 -1.83447
C 7.70798 -1.39369 1.9661
C -1.21523 6.16529 -1.88047
C 6.41542 -1.41168 1.3368
C -6.12375 0.74891 1.42363
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C -6.34677 -1.6802 1.36982
C -5.83082 -2.90749 0.88349
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C -4.07583 -6.23852 -1.19463
C -7.67175 -1.53616 1.87405
C -7.46703 0.86651 1.82298

H -8.23376 -2.45792 1.98913
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H 7.48414 3.439 1.68363
H 8.25759 -2.33294 1.96876
C 5.62057 -0.1993 1.30419
N -0.81978 1.94965 0.03195
N -2.26786 -1.86185 0.55723
N -5.53754 -0.52758 1.33202
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C -1.89992 -5.10642 -1.08937
C 5.92675 -2.57485 0.70267
C -6.09167 3.10133 0.76373
C -3.4742 5.13664 -1.10744
C -0.235 -2.96422 -0.00699
H -2.38314 0.40514 0.73221
H 0.025 -1.97072 -0.51475
O 0.24414 -3.00765 1.3214
H 1.1072 -2.55681 1.3608
O -2.92408 0.80561 2.62268
H -3.68825 1.11992 3.1307
O 4.10763 -6.77682 -1.91001
H 5.07277 -6.84465 -1.83065
O 7.83849 -4.05703 0.75163
O 7.93578 1.97366 3.14046
O -7.87599 -4.20261 1.03395
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N 1.71168 -4.10361 -0.98487
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C -7.42045 3.22184 1.25332
C -2.09039 -7.26008 -2.28722
C -0.75455 -7.25056 -2.5397
C 3.02117 5.86242 -1.22465
C 1.12563 7.15646 -2.10617
C 2.46693 7.04659 -1.81
C 4.34901 5.78893 -0.73315
O 5.11582 6.87682 -0.90108
H 6.00418 6.75288 -0.5319
C -6.17821 5.29397 -0.35556
C -4.27524 6.2216 -1.48252
H -3.83534 7.02406 -2.0641
C -5.61927 6.30023 -1.11476
O -1.7921 7.30613 -2.32667
H -6.2207 7.15769 -1.42317
H -7.22626 5.36982 -0.07516
H -7.94351 4.17387 1.19332
H -9.10051 2.24327 2.16517
H -9.22163 -0.2118 2.52223
H -6.68911 -6.04476 -0.29848
H -4.67192 -7.09564 -1.5165
H -2.71764 -8.07941 -2.64495
H -0.28366 -8.06331 -3.09657
H 1.94979 -7.13024 -2.56098
H 6.44442 -5.80486 -0.51098
H 9.16929 -0.28685 3.08025
H 6.75803 5.42199 0.51997
H 3.12636 7.89608 -1.98838
H 0.76852 8.10488 -2.51557
H -1.12043 7.95824 -2.57675
Pd 1.00922 -0.37204 -0.17138

NSPC-Pd^{II}

0 1

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C -2.81541 -5.7345 1.12008
C -1.80125 -6.478 0.49671
C -5.04008 -5.16896 2.03846
C -4.06399 -6.10897 1.72606
C 2.49586 -2.07642 0.04586
C 3.48178 -2.96836 -0.51058
C 1.7474 -4.66373 -0.91616
C 0.75164 -3.84198 -0.38738
C -1.56146 -3.64928 0.39403
C -2.61027 -4.35671 1.02302
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C -4.06973 -1.17178 0.56896
C -3.14242 -2.2002 0.72156
C -6.40457 -0.44148 0.62979
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C -7.79286 -0.58411 1.12715
C 4.11602 -0.5027 0.51207
C 3.17064 1.7473 0.5756
C 4.35691 0.84665 0.72403

C -3.63897 0.07578 -0.15043
C -4.70695 1.09947 -0.38153
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C -7.09028 1.40352 -0.87101
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C 3.9733 5.89364 1.36956
C 3.45999 3.16578 0.9054
C 2.39445 4.08767 0.79034
C 2.68005 5.48252 0.98379
C 0.19588 4.47441 0.12965
C 0.42848 5.93941 0.1983
C -1.11594 4.05138 -0.28907
C -1.98381 5.08685 -0.65339
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C 4.84313 -2.59968 -0.43559
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C 8.24732 2.21453 1.38269
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N -1.85203 -2.34291 0.21855
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C 3.10928 -4.21089 -1.04053
C -4.89968 -3.75027 1.68916
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C 1.65405 6.3895 0.67531
C 1.0294 -2.41719 -0.01869
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H 0.53617 -2.15805 0.92321
O 2.73163 1.6327 -0.78807
H 1.77159 1.82118 -0.75921
O -1.8168 -7.82679 0.37378
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O -6.16306 -5.65165 2.644
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O 8.85206 -1.50295 -0.12346
C -3.20006 4.50062 -0.99753
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H -7.32873 4.77838 -2.151
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H 8.01472 -3.67713 -1.18864
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SPC-Pd^{II}

2 1

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C -5.29788 -4.28641 2.59514
C -4.22906 -5.14363 2.79833
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C -3.78051 -2.71643 1.6042
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H -1.58998 -1.20254 2.06815
H -7.06811 -3.89043 3.247
Pd -1.4709 -0.58279 -1.82742

$Pd(NO_3)_2$

0 1

Pd 0. -0.00036 0.
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O 1.77436 1.05977 0.
O -1.76568 1.07594 0.
N -2.48802 0.01097 0.
N 2.48799 -0.01057 0.
O -1.77518 -1.05964 0.
O -3.68041 0.01603 0.
O 3.68039 -0.01459 0.

NO_3^-

-1 1

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O 0. 0. 1.25161
O 0. 1.08464 -0.62568
O 0. -1.08464 -0.62568

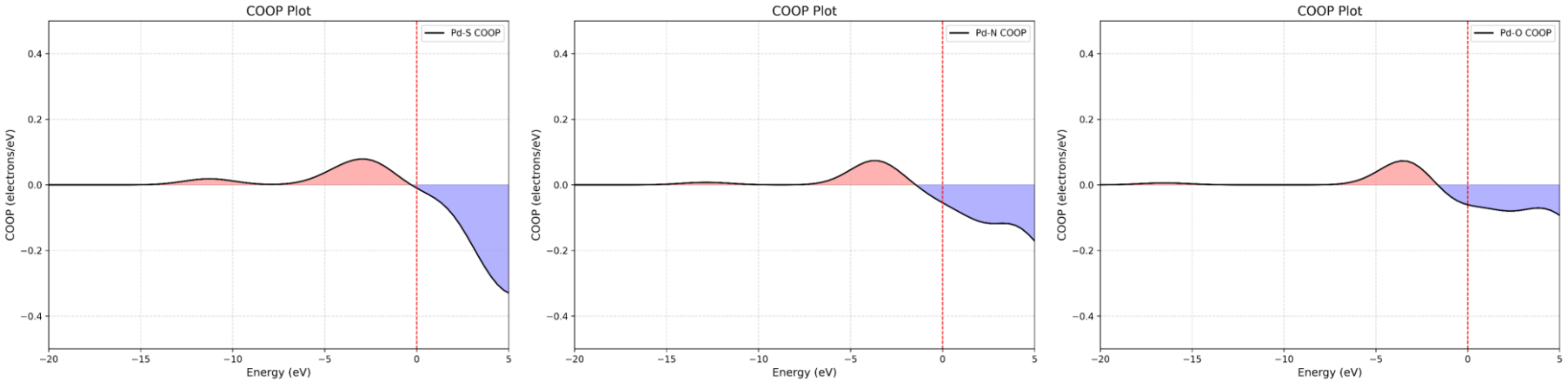

Figure S1. The bonding strengths for Pd-S, N, and O atoms.

Crystal Orbital Overlap Population (COOP) is a computational tool for analyzing chemical bonding characteristics between atomic orbitals. The COOP function describes the density of states of overlapping orbitals between two atomic orbitals, combining both density of states (DOS) and interorbital overlap integrals. In the energy region below the Fermi level (x < 0 eV), COOP reflects the bonding interactions between atoms, where COOP > 0: Indicates bonding states COOP < 0: Indicates antibonding states. The COOP analysis reveals distinct bonding strengths for Pd-X interactions (X = S, N, O). The integrated COOP (I_{COOP}) values confirm the hierarchy: Pd-S (9.796 eV) > Pd-N (6.062 eV) > Pd-O (4.539 eV), consistent with HSAB-principle predictions.

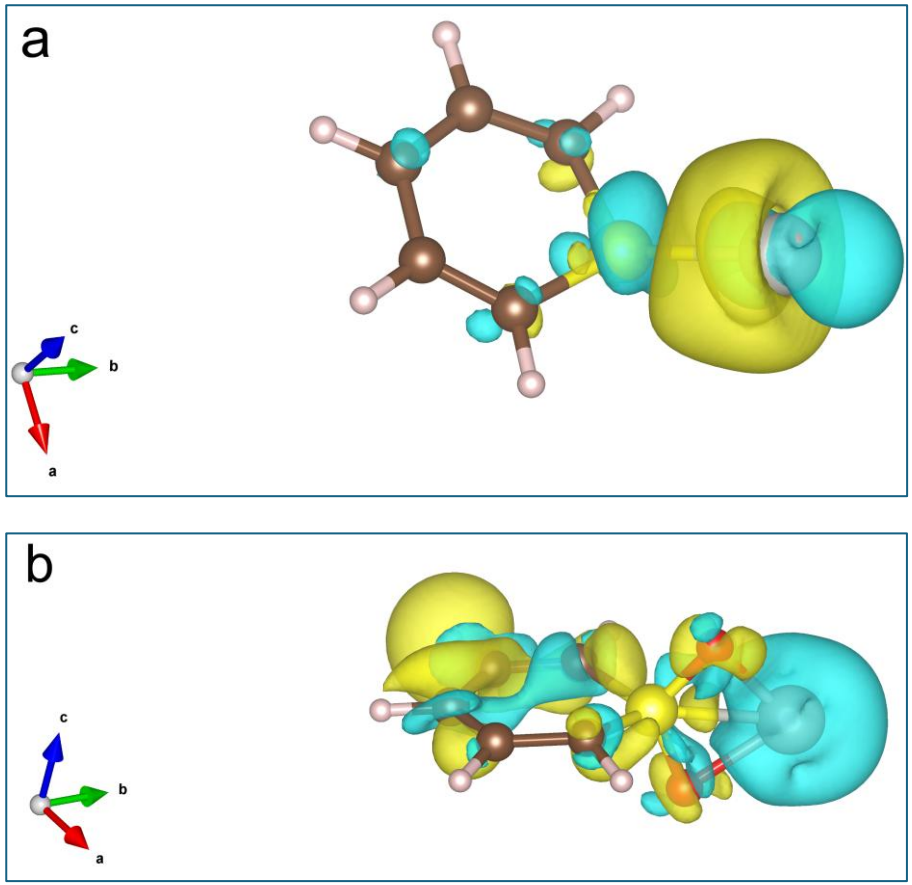

Figure S2. Bader charge analysis of a) C-S-C and b) C-SO_x on NSPC for Pd(II) adsorption (The yellow area represents the aggregation of electrons, and the blue area represents the disappearance of electrons).

Bader charge analysis reveals distinct electron transfer behaviors in the system. As shown in Figure S2a, electrons from the C-S-C moiety preferentially transfer to Pd, with a calculated charge transfer of 0.2796 e^-. Conversely, Figure S2b demonstrates that Pd acts as an electron donor to S

in C-SO_x, facilitating a more substantial electron transfer of 0.3223 e^-.

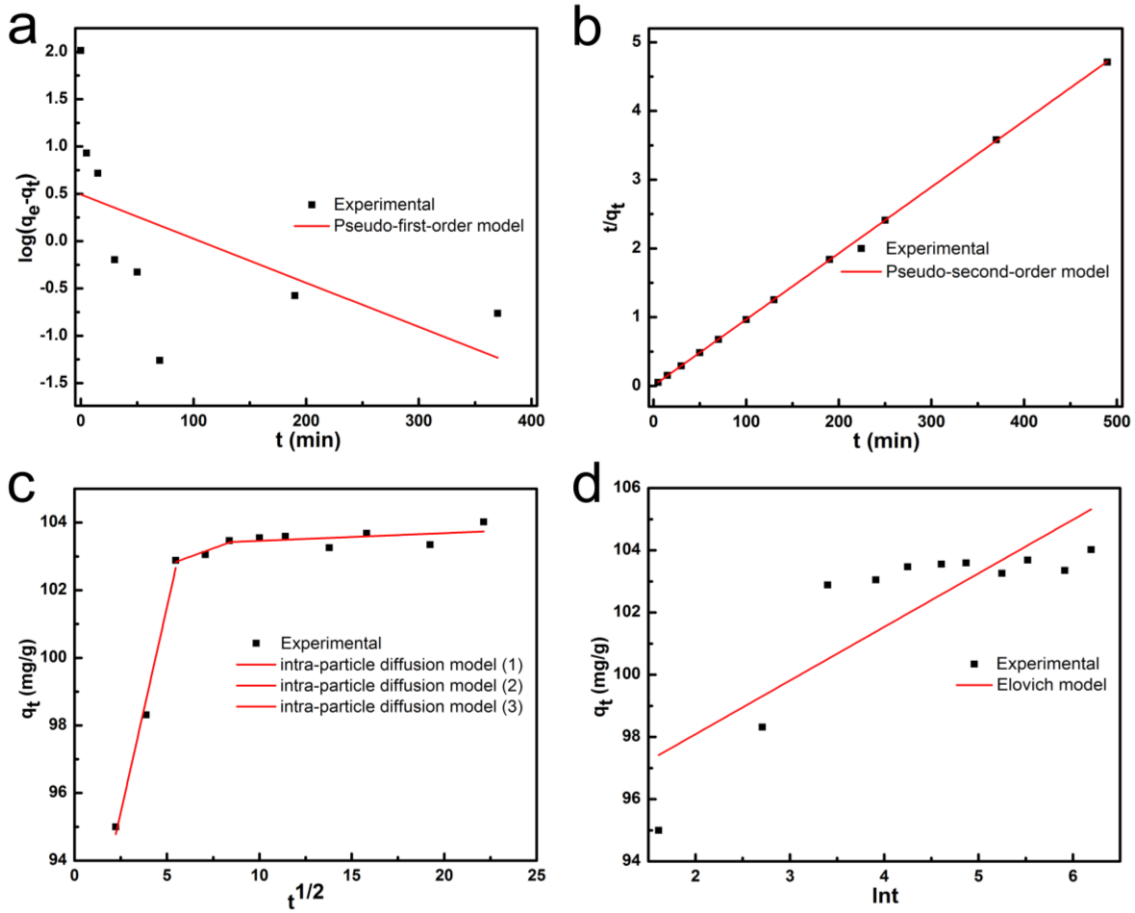

Figure S3. Adsorption kinetics of Pd(II) on NSPC. a) Pseudo-first-order model; b) Pseudo-second-order model; c) intra-particle diffusion model; d) Elovich model

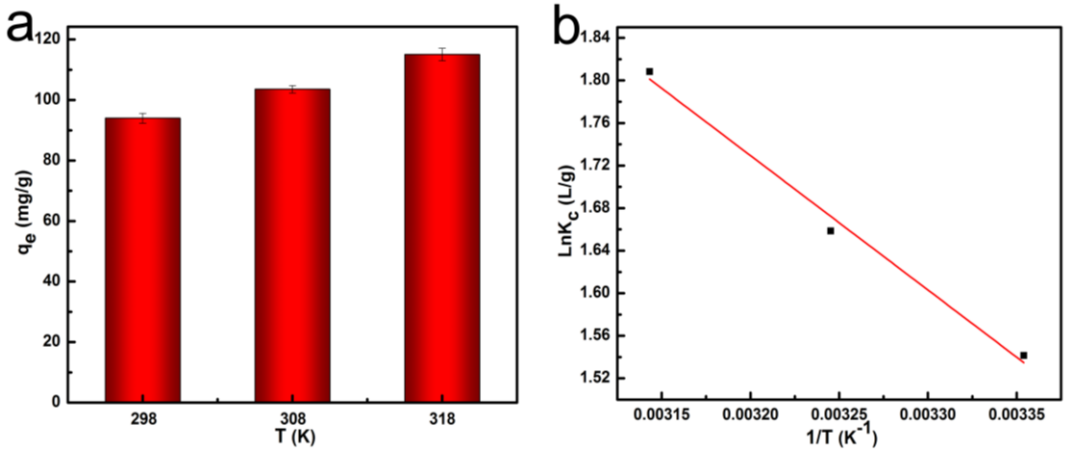

Figure S4. a) Adsorption capacity of Pd(II) on NSPC at different temperatures; b) Van't Hoff diagram of lnKc-1/T ([NSPC]=200 mg L^{-1}, Pd(II)=40 mg L^{-1}, [HNO_3]=1 mol L^{-1}).

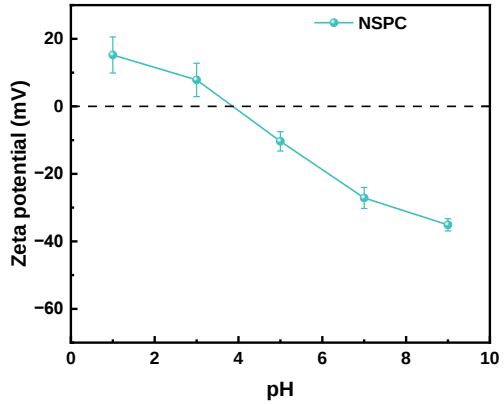

Figure S5. pH-dependent Zeta potential of NSPC.

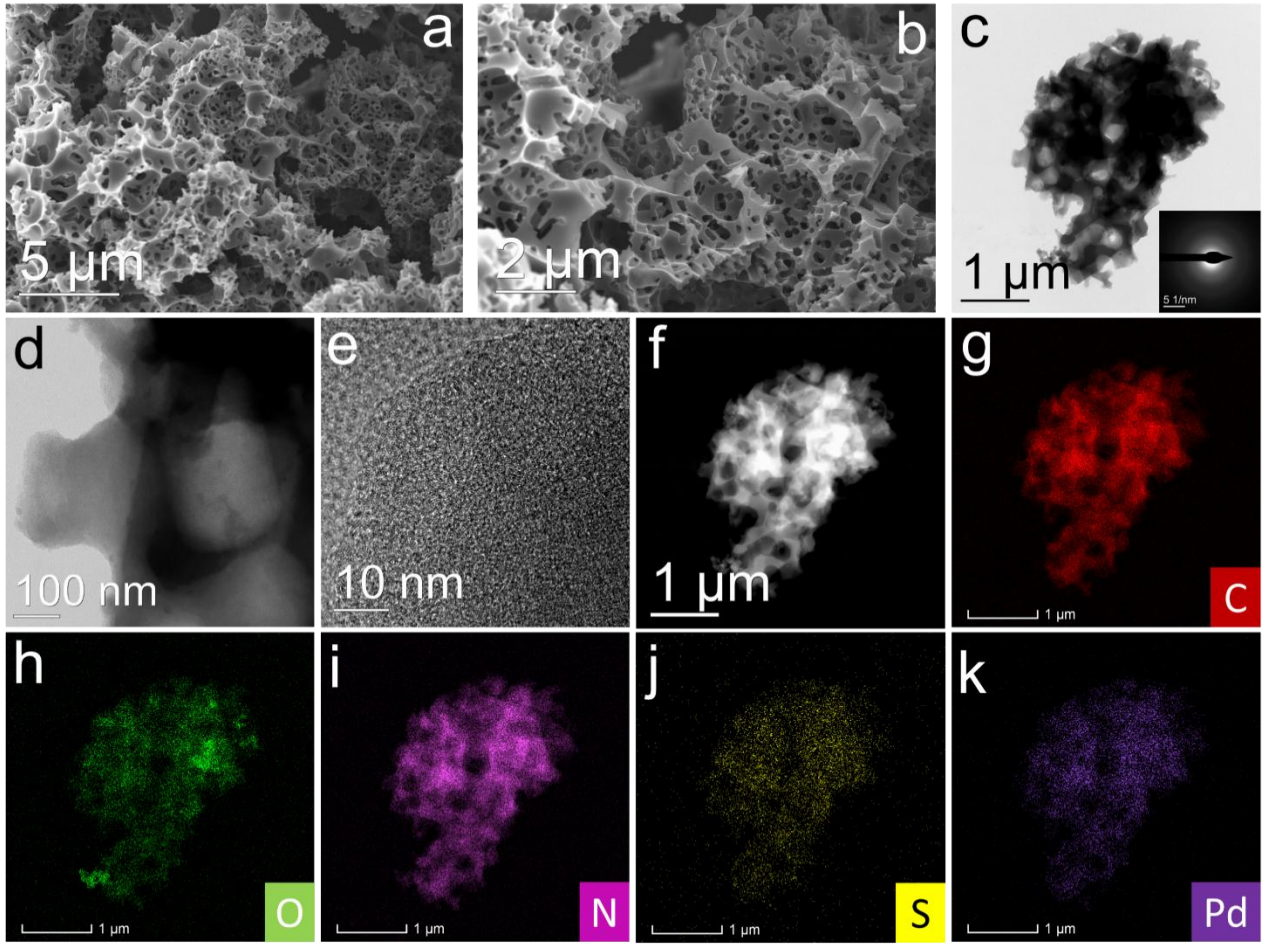

Figure S6. a, b) SEM, c) TEM and SAED (inset), d, e) HRTEM, f) HAADF, g-k) EDS mapping images of used NSPC.

Table S1. Specific surface area and pore volume of as-prepared porous carbon materials

Sample	Surface area* ($m^2\ g^{-1}$)	Pore volume** ($cm^3\ g^{-1}$)
SPC	1502	0.68
NPC	2539	1.18
NSPC	1932	0.86

*using the Brunauer-Emmett-Teller (BET) method

**using the Horvath-Kawazoe (HK) method

Table S2. The detailed calculation of the adsorbent price

No.	Sorbent	Reagent	Unit cost (RMB/g or mL)	Dosage (g or mL)	Cost (RMB)	Source	Calculation formula	Sorbent Price* (RMB/g)	Ref
1	C_8-Cyclen/CG-71M	CG-71M resins	11.1	1	11.1	Thermo Scientific	C_8-Cyclen = (1940.16+15.36+9.49)/2.06g=953.9 RMB C_8-Cyclen/CG-71M = (1g CG-71M+0.2g C_8-Cyclen)/1.2g =168.3 RMB	168.3	14
		Cyclen	1128	1.72	1940.16	Sigma Aldrich			
		NaH	8	1.92	15.36	Thermo Scientific			
		1-bromo-octane	1.15	8.29	9.49	Thermo Scientific			
2	CA-BOPhen SiO_2-P	2,9-Dimethyl-1,10-phenanthroline	163.4	10	1634	Alfa Aesar	2,9-Dicarbaldehyde-1,10-phenanthroline 9.9 g = (1634+26.6)/9.9g =167.7RMB/g	257.6	15
		SeO_2	1.9	14	26.6	MACKLIN			
		Hydroxylamine hydrochloride	0.57	6.1	3.477	Thermo Scientific	2,9-dicarbonitrile-1,10-Phenanthroline = (9.6 g 2,9-Dicarbaldehyde-1,10-phenanthroline +3.477+18.278+2.8016)/4 = 408.6 RMB/g		
		p-Toluenesulfonyl chloride	0.74	24.7	18.278	Alfa Aesar			
		pyridine	0.136	20.6	2.8016	Alfa Aesar			
		Hydrazine hydrate	1.148	91	104.5	ALADDIN	2,9-dicarbohydrazonamide-1,10-phenanthroline = (3.88g 2,9-dicarbonitrile-1,10-Phenanthroline + 104.5)/3.5g =482.8 RMB/g		
		Camphoroquinone	39.91	4.5	179.6	Alfa Aesar	CABOPhen = (3.5*482.8+179.6)/1.3g= 1438 RMB/g		
		SiO_2-P	1.9856	4.5	8.935	Honeywell Chemicals	CA-BOPhen SiO_2-P = (0.8 g CABOPhen+ 8.935)/4.5g=257.6RMB/g		
3	HEMAP/Si O_2-P	Porous SiO_2	29.2	50	1460	Thermo Scientific	SiO_2-P= (1460+46.34+2.1+3.39+2.4+2.89+3.59)/50g = 30.4 RMB/g	53.4	16
		Diethyl phthalate	3.11	14.9	46.34	Alfa Aesa			
		1,1'-Azobis (cyanocyclohexane)	19.1	0.11	2.1	Sigma Aldrich			
		Styrene	0.372	9.1	3.39	Alfa Aesar			
		Divinylbenzene	0.08	30	2.4	Macklin			
		hypnone	0.124	23.3	2.89	Macklin			
		AIBN	22.43	0.16	3.59	Sigma Aldrich			
		2-Hydroxyethyl methacrylate phosphate	46	5	230	Macklin	HEMAP/SiO_2-P = (10g*30.4+230)/10g = 53.4 RMB/g		
4	Tp-Azo-COF/SiO_2	SiO_2	1.714	4	6.856	Honeywell Chemicals	Tp-Azo-COF/SiO_2 = (6.856+129.2+125.8+14.97+7.878)/4g	71.1	17

		Tp	586	0.2205	129.2	Thermo Scientific	= 71.1 RMB/g		
		Azo	376.44	0.3342	125.8	Thermo Scientific			
		o-DCB	0.998	15	14.97	Thermo Scientific			
		DMAC	0.525	15	7.875	Thermo Scientific			
5	Si-TpAL	3-aminopropyl -functionalized silica-gel	64.811	1	64.81	Sigma Adrich	Si-TpAL = (64.81+146.5+16.2)/1g = 227.5 RMB/g	227.5	18
		1,3,5-triformyl phloroglucinol	586	0.25	146.5	Thermo Scientific			
		1,4-Dioxane	0.36	45	16.2	Thermo Scientific			
6	NTAamide(C8) /SiO_2-P	SiO_2	1.714	10	17.14	Honeywell Chemicals	NTAamide(C8)/SiO_2-P = (17.14+4.11+31.86+4.49+3.82+1000)/10g = 104.4 RMB/g	104.4	19
		styrene	1.246	3.3	4.11	Thermo Scientific			
		divinylbenzene	10.62	3	31.86	Thermo Scientific			
		AIBN	22.43	0.2	4.49	Sigma Aldrich			
		V-40	19.1	0.2	3.82	Sigma Aldrich			
		NTAamide(C8)(95%)	200	5	1000.00	Merck			
7	2AT-SiAaC	AA	0.333	2.2	0.7326	Thermo Scientific	2AT-SiAaC = (0.7326+0.9856+4.13+1.12+12)/7g= 2.7 RMB/g	2.7	20
		DMSO	0.448	4	0.9856	Thermo Scientific			
		EGDMA	5.162	0.8	4.13	Thermo Scientific			
		AIBN	22.43	0.05	1.12	Sigma Aldrich			
		SiO_2	1.714	7	12.00	Honeywell Chemicals			
8	MBT/XAD7HP	Amberlite XAD7HP	3.482	3.75	13.06	Thermo Scientific	MBT/XAD7HP= (13.06+2.206)/3.75=4.1 RMB/g	4.1	21
		MBT	1.765	1.25	2.206	Thermo Scientific			
9	CTF-S	Chloroacetonitrile	11.2	1.54	17.248	Thermo Scientific	IL-S = (17.248+240.38)/1.65g=156.1 RMB/g	225.4	22
		1,4-Bis(1-imidazolyl)benzene	238	1.01	240.38	Macklin			
		anhydrous ZnCl2	2.98	3.82	11.38	Thermo Scientific	CTF-S=(1.01g IL-S+3.82g ZnCl2)/0.75g =225.4 RMB/g		
10	Si@-UiO−SO_3H MOF	$ZrCl_4$	6.830	5.47	37.36	Thermo Scientific	Sorbent =(37.36+2.83+323.76+105.75+7.6+59.17)/4.35g = 123.3RMB/g	123.3	23
		H_2BDC	0.880	3.22	2.83	Thermo Scientific			
		2-$NaSO_3$-H_2BDC	54.782	5.91	323.76	TCI America			
		N, N dimethylformamide	0.423	250	105.75	Thermo Scientific			
		Acetic acid	0.19	40	7.6	Thermo Scientific			
		Silica	13.6	4.35	59.17	Fisher Chemica			
11	COP-2	SeO_2	1.9	8	15.2	Macklin	Phen-CHO = (15.2+58+817)/2.3g	530	24

		1,4-dioxane	0.232	250	58	Macklin	=387.1 RMB/g		
		2,9-dimethyl-1,10-phenanthroline	163.4	5	817	Thermo Scientific			
		4-Aminobenzonitrile	32.4	2	64.8	Thermo Scientific	TAPT= (64.8+296.7)/1.41g=256.4 RMB/g		
		trifluoromethanesulfonic acid	34.3	8.65	296.7	Thermo Scientific			
		1-butanol	0.77	20	15.4	Thermo Scientific	COF-1=(387.1+256.4+15.4+23.8)/1.62g = 421.4 RMB/g		
		o-dichlorobenzene	1.19	20	23.8	Thermo Scientific			
		dry Oxone	3.84	1.86	7.14	Thermo Scientific	COF-2= (0.45g COF-1+7.14+25.84)/0.42 =530 RMB/g		
		dry DMF	1.52	17	25.84	Thermo Scientific			
12	CN-DAPhen	Oxalic acid	1.89	1	1.89	Thermo Scientific	CN-DAPhen= (1.89+0.9+511.5+52.5+4.3+0.22+1.13)/1.4g =408.9 RMB/g	408.9	25
		Melamine	0.452	2	0.90	Thermo Scientific			
		1,10-phenanthroline-2,9-dicarboxylic acid	3410	0.15	511.5	Thermo Scientific			
		thionyl chlorid	3.5	15	52.50	ALADDIN			
		Dichloromethane	0.086	50	4.30	Thermo Scientific			
		Triethylamin	0.374	0.6	0.22	Thermo Scientific			
		N-ethyl-p-toluidine	2.516	0.45	1.13	ALADDIN			
13	P_5COP-m-BPT	P5A-N3	0.8436	1.5	1.27	www.ansitan.com	P_5COP-m-BPT=(1.27+2334+0.92+0.12+34.49)/2.35g =1008.9 RMB/g	1008.9	26
		6,6′-Diethynyl-3,3′-bipyridine	1995	1.17	2334	Jilin Chinese Academy of Sciences - Yanshen Technology Co., Ltd.			
		Sodium ascorbate	2.020	0.456	0.92	Thermo Scientifi			
		$CuSO_4$ $5H_2O$	1.714	0.072	0.12	Thermo Scientifi			
		DMF	0.345	100	34.49	Thermo Scientifi			
14	SBA-15-TEPA	SBA-15	113	2.2	248.6	ALADDIN	SBA-15-TEPA= (248.6+0.0785+4.61+19.76)/2.2g=124.1 RMB/g	124.1	27
		30%Hydrogen Peroxide	0.157	0.5	0.0785	ALADDIN			
		Tetraethylenepentamine	1.522	3.03	4.61	Thermo Scientifi			
		(3-Chloropropyl) trimethoxysilane	6.63	2.98	19.76	Thermo Scientifi			
15	SBA-IL	N-methyl-N′-propylimidazole	1.570	6.57	10.31	Alfa Aesar	SBA-IL = (10.31+105.35+226)/2g = 170.8RMB/g	250.4	28
		3-chloropropyl trimethoxysilane	6.63	15.89	105.35	Thermo Scientific			
		Mesoporous SBA-15	113	2	226	ALADDIN			

16	NSPC	Glucose, anhydrous	0.118	6.5	0.77	Thermo Scientific	Hydrothermal carbon=(0.77+1.47)/3.86g =0.58 RMB/g NSPC=(0.58+0.22+0.06)/0.24g=3.5 RMB/g	3.5	This work
		Melamine	0.452	3.25	1.47	Alfa Aesar			
		Potassium hydroxide	0.072	3	0.22	Macklin			
		Ammonium sulfate	0.283	0.2	0.06	Alfa Aesar			

*The value of the main raw materials consumed in the preparation process of 1g of adsorbent was calculated. The common solvents required for preparing the reaction solution and used in the sample washing process, as well as the instruments, equipment and labor were not considered.

Table S3. Kinetic model parameters of Pd(II) adsorption on NSPC.

Kinetic model	Parameters		
Pseudo-first-order model	q_e	k_1	R^2
	3.11	0.0107	0.196
Pseudo-second-order model	q_e	k_2	R^2
	103.9	0.0173	0.999
Intra-particle diffusion model	C_1	k_{i1}	R_1^2
	89.3	2.43	0.981
	C_2	k_{i2}	R_2^2
	101.8	0.198	0.824
	C_3	k_{i3}	R_3^2
	103.2	0.0227	0.0464
Elovich model	α_E	β_E	R^2
	1.21×10^{24}	0.580	0.685

Table S4. Isotherm model parameters of Pd(II) adsorption on NSPC.

Adsorption model	Parameters		
Langmuir	q_{max}	k_L	R^2
	248	0.0325	0.824
Freundlich	n	k_F	R^2
	3.46	46.1	0.988
Temkin	b	k_T	R^2
	88.2	4.12	0.847

Table S5. Thermodynamic parameters of Pd(II) adsorption on NSPC

Temperature（K）	ΔG（kJ mol^{-1}）	ΔH（kJ mol^{-1}）	ΔS（J $mol^{-1}K^{-1}$）
298	-3.80		
308	-4.28	10.5	48.0
318	-4.76		

Table S6. The concentration, distribution coefficient Kd and selectivity coefficient K of various metal ions in HNO_3 solution (1/2/3 M)

Ions	Conc. (mg L^{-1})	K_d (mL g^{-1})			K		
		1 M	2 M	3 M	1 M	2 M	3 M
Pd	26.21	2.9×10^3	2.0×10^3	1.6×10^3			
Mo	16.44	1.6×10^2	1.6×10^2	17.8	1.8×10^1	1.2×10^1	8.8×10^1
Na	20.79	1.0×10^2	0	0	2.8×10^1	$>2.0\times10^4$	$>1.6\times10^4$
Nb	16.52	1.1×10^2	83.3	0	2.6×10^1	2.4×10^1	$>1.6\times10^4$
Ru	15.22	97.9	95.2	18.8	3.0×10^1	2.1×10^1	8.3×10^1
K	5.29	2.7×10^2	0	0	1.1×10^1	$>2.0\times10^4$	$>1.6\times10^4$
Al	14.37	80.4	0	0	3.6×10^1	$>2.0\times10^4$	$>1.6\times10^4$
Cu	13.75	79.4	41.6	36.4	3.6×10^1	4.7×10^1	4.3×10^1
Pb	15.18	33.4	31.9	25.1	8.7×10^1	6.2×10^1	6.2×10^1
Zr	12.60	35.2	25.3	0	8.2×10^1	7.8×10^1	$>1.6\times10^4$
Li	12.97	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Mg	14.52	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Ca	42.01	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Ti	15.22	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Cr	16.20	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Mn	13.15	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Fe	20.70	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Co	14.51	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Ni	12.96	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Zn	19.68	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Cd	15.75	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Ba	15.33	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
La	13.20	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Ce	15.58	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$
Nd	14.75	0	0	0	$>2.9\times10^4$	$>2.0\times10^4$	$>1.6\times10^4$

Table S7. EXAFS fitting parameters at the Pd K–edge for Pd samples

Sample	Shell	CN[a]	R(Å)[b]	σ^2(Å^2)[c]	ΔE_0(eV)[d]	K-range/Å^{-1}	R-range/Å	R factor
Pd foil	Pd-Pd	12.0*	2.74±0.01	0.0054±0.0003	-5.6±0.2	2-12	1.0-3.0	0.0021
PdO	Pd-O	4.0±0.3	2.02±0.01	0.0014±0.0006	9.2±0.6	2-12	1.0-3.7	0.0053
	Pd-Pd	4.7±1.0	3.05±0.01	0.0050±0.0014	8.1±1.0			
	Pd-Pd	5.8±1.5	3.43±0.01	0.0042±0.0016	7.2±0.7			
Pd-NSPC	Pd-O	2.2±0.2	2.01±0.01	0.0032±0.0008	2.6±0.6	2-12	1.0-3.0	0.0049
	Pd-S	0.2±0.1	2.36±0.01	0.0031±0.0005	8.9±4.0			
	Pd-Pd	2.3±0.5	2.71±0.01	0.0118±0.0014	-4.9±0.9			

[a]CN, coordination number; [b]R, distance between absorber and backscatter atoms; [c]σ^2, Debye-Waller factor to account for both thermal and structural disorders; [d]$\Delta E(0)$, inner potential correction; R factor indicates the goodness of the fit. S_0^2 was fixed to 0.809, according to the experimental EXAFS fit of **Pd** foil by fixing CN as the known crystallographic value. A reasonable range of EXAFS fitting parameters: $0.700 < S_0^2 < 1.000$; CN > 0; σ^2Å$^2 > 0$; $|\Delta E_0| < 15$ eV; R factor < 0.02.

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