**Supplementary Material**

**Theoretical design of azaacene-based non-fullerene electron transport material used in inverted perovskite solar cells**

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**TABLE S1** The predicted point group and crystalline cell parameters of compounds **1-3** and **NDI-PM**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compounds | **1** | **2** | **3** | **NDI-PM** | **NDI-PM Expt.** |
| Point Group | *P*1 | *P*1 | *P*21 | *P*1 | *P*1 |
| *a*/Å | 18.1364 | 23.0347 | 12.1911 | 8.3500 | 8.3500(3) |
| *b*/Å | 7.6560 | 8.7787 | 23.8509 | 8.6060 | 8.6060(4) |
| *c*/Å | 35.6185 | 21.0868 | 14.5643 | 15.3260 | 15.3260(7) |
| *α*/(°) | 70.0537 | 29.0716 | 90.0000 | 98.5520 | 98.5520(12) |
| *β*(°) | 74.9956 | 62.7198 | 108.1955 | 102.7330 | 102.7330(10) |
| *γ*(°) | 56.4569 | 77.0295 | 90.0000 | 92.1280 | 92.1280(11) |

NDI-PM.tif

**FIGURE S1** The sketch structure of **NDI-PM**.

opt-NDI-PM-transfer-pathways.tif

**FIGURE S2** The transfer pathways of the tested molecule **NDI-PM**.

**TABLE S2** The centroid to centroid distances (*r*, Å), the calculated reorganization energy (*λ*, eV), the calculated electronic couplings (*V*, meV), charge transfer rate (*k*, s−1)and electron mobility (*µ*, cm2·V−1·s−1) during the electron transport process based on the optimized crystal structure

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound | λ | Pathway | *r* | *V* | *k* | *µ* |
| **NDI-PM** | 0.29 | 1 | 4.18 | -95.81 | 1.80×1013 | 0.20 |
| 2 | 9.43 | -0.13 | 3.39×107 |
| 3 | 8.61 | -17.18 | 5.78×1011 |
| 4 | 9.70 | 10.11 | 2.00×1011 |
| 5 | 8.35 | -5.32×10-3 | 5.55×104 |
| 6 | 11.77 | 7.33×10-3 | 1.05×105 |

The optimized geometries of the ground state in Cartesian coordinates:

Compound **1**

6 -0.117928 -2.422709 -0.070531

6 0.600123 -1.229269 -0.052714

6 -0.136814 -0.026186 -0.034779

6 -1.504668 -0.019014 -0.036536

6 -2.255548 -1.212519 -0.053221

6 -1.551148 -2.414065 -0.070055

6 0.611434 1.169659 -0.019150

6 -0.093195 2.370902 -0.006274

6 -1.526041 2.377283 -0.010110

6 -2.242101 1.182769 -0.025536

6 2.005326 -0.779103 -0.048603

6 2.011561 0.706765 -0.025930

6 -3.656170 -0.741673 -0.050239

6 -3.647247 0.728061 -0.038006

7 3.096966 -1.482693 -0.062974

6 4.279949 -0.769231 -0.057191

6 4.285069 0.679920 -0.033382

7 3.108126 1.402213 -0.016828

7 -4.745367 1.436272 -0.042319

6 -5.916240 0.724557 -0.055523

6 -5.925478 -0.708647 -0.054769

7 -4.763545 -1.435708 -0.054930

6 5.487095 -1.492751 -0.072801

6 6.729721 -0.774278 -0.080472

6 6.734293 0.672888 -0.053029

6 5.495926 1.396895 -0.024584

6 -7.153631 1.446113 -0.069581

6 -8.348380 0.725241 -0.075887

6 -8.357730 -0.674496 -0.064795

6 -7.173157 -1.412293 -0.052704

7 7.877995 -1.471434 -0.112328

6 9.022152 -0.780788 -0.114381

6 9.026706 0.667268 -0.082033

7 7.886691 1.364197 -0.052810

6 10.269503 -1.479214 -0.148439

6 11.445479 -0.779203 -0.148577

6 11.450008 0.651588 -0.115362

6 10.278562 1.358432 -0.083274

6 5.489428 -2.908528 -0.076777

6 5.503232 -4.130278 -0.073382

14 5.539507 -5.971822 -0.094396

6 5.502219 2.811875 0.019919

6 5.512830 4.032513 0.069941

14 5.536301 5.871838 0.185557

6 -7.204844 -2.833848 -0.029936

6 -7.257994 -4.053980 0.002502

14 -7.213582 -5.897835 0.054862

6 -7.160963 2.868167 -0.075011

6 -7.184114 4.089666 -0.080314

14 -7.077010 5.931613 -0.042829

6 3.750002 -6.599657 -0.423073

6 6.731082 -6.513928 -1.500904

6 6.313797 -6.539096 1.569400

6 4.746814 6.533076 -1.433725

6 7.374088 6.407550 0.276701

6 4.643820 6.309722 1.827805

6 -7.197770 -6.459453 1.894347

6 -8.738673 -6.553714 -0.898980

6 -5.589947 -6.402171 -0.832810

6 -5.602008 6.326359 1.118212

6 -8.713411 6.605155 0.689820

6 -6.743812 6.565341 -1.826672

6 2.983504 -5.687497 -1.404747

6 2.906500 -6.798995 0.851029

6 8.129158 -5.883693 -1.339006

6 6.188758 -6.247330 -2.917370

6 6.393771 -8.072431 1.711454

6 5.704534 -5.893191 2.828103

6 4.774911 8.068868 -1.559770

6 3.336928 5.982683 -1.721951

6 8.161153 6.000681 -0.984486

6 8.072588 5.862798 1.537719

6 3.203250 5.771763 1.918489

6 4.699482 7.805308 2.194674

6 -7.680982 -7.913012 2.079018

6 -7.951027 -5.513469 2.849247

6 -8.670541 -6.220887 -2.402210

6 -10.068411 -6.054882 -0.300578

6 -5.380434 -7.926368 -0.916297

6 -4.353201 -5.708633 -0.229345

6 -5.387649 7.831727 1.367001

6 -4.295344 5.654335 0.653110

6 -8.904926 6.180767 2.158667

6 -9.945141 6.208641 -0.147135

6 -7.112840 8.052207 -2.010339

6 -7.386492 5.708404 -2.934387

1 0.397686 -3.378263 -0.087397

1 -2.077240 -3.364016 -0.085370

1 0.433712 3.320290 0.005886

1 -2.042938 3.332322 -0.000343

1 -9.287706 1.268330 -0.086736

1 -9.304354 -1.204865 -0.064298

1 10.239386 -2.563935 -0.173092

1 12.393648 -1.308985 -0.174066

1 12.401520 1.175960 -0.116343

1 10.255737 2.443324 -0.058517

1 3.867954 -7.585702 -0.900952

1 6.839212 -7.605053 -1.390082

1 7.347427 -6.167541 1.496931

1 5.411159 6.129073 -2.213394

1 7.377878 7.507297 0.336895

1 5.235619 5.766288 2.580819

1 -6.135153 -6.428205 2.181702

1 -8.714531 -7.649910 -0.796116

1 -5.705804 -6.024741 -1.859954

1 -5.877938 5.866660 2.079160

1 -8.630450 7.702847 0.665079

1 -5.652744 6.480902 -1.947710

1 3.495243 -5.573585 -2.365326

1 2.854439 -4.682359 -0.986398

1 1.985999 -6.101202 -1.610020

1 2.779953 -5.856697 1.398141

1 3.348992 -7.526375 1.539057

1 1.901889 -7.161766 0.592507

1 8.603487 -6.163193 -0.391452

1 8.076426 -4.788842 -1.372041

1 8.796862 -6.211207 -2.147767

1 6.003168 -5.178540 -3.080323

1 5.253395 -6.783541 -3.110691

1 6.914185 -6.571673 -3.676209

1 6.951697 -8.349116 2.616463

1 5.399510 -8.527698 1.797911

1 6.899675 -8.544771 0.860844

1 6.296769 -6.151207 3.716978

1 5.679252 -4.801044 2.750091

1 4.681144 -6.237552 3.011704

1 5.777838 8.483186 -1.403708

1 4.104253 8.545474 -0.834706

1 4.442781 8.382269 -2.558884

1 2.594816 6.396874 -1.029299

1 3.298336 4.891038 -1.639020

1 3.016048 6.254447 -2.737148

1 9.207361 6.328770 -0.911693

1 8.164759 4.911005 -1.110726

1 7.744504 6.441145 -1.897705

1 9.121980 6.186914 1.571463

1 7.594545 6.208392 2.461419

1 8.065846 4.766003 1.547792

1 2.807589 5.894130 2.936162

1 2.529447 6.313953 1.244298

1 3.148363 4.707821 1.662789

1 4.286665 7.973707 3.198830

1 5.722997 8.198463 2.192591

1 4.109965 8.414643 1.499278

1 -7.126047 -8.624663 1.457410

1 -8.744023 -8.018506 1.829759

1 -7.562275 -8.229464 3.124192

1 -9.025659 -5.488382 2.630957

1 -7.579213 -4.486334 2.781569

1 -7.839408 -5.846850 3.890184

1 -7.787563 -6.654453 -2.884901

1 -8.640811 -5.136961 -2.568768

1 -9.554679 -6.608540 -2.926493

1 -10.132508 -4.960515 -0.337444

1 -10.194667 -6.357694 0.744836

1 -10.923238 -6.453685 -0.863856

1 -4.493425 -8.165820 -1.518514

1 -5.220183 -8.364144 0.076811

1 -6.234111 -8.442394 -1.372217

1 -3.452614 -5.951151 -0.811312

1 -4.467491 -4.618960 -0.214579

1 -4.168410 -6.040712 0.800663

1 -6.294264 8.329612 1.731541

1 -5.068713 8.349709 0.453800

1 -4.601423 7.994088 2.116889

1 -3.945280 6.074568 -0.299034

1 -4.421624 4.574296 0.517739

1 -3.495048 5.814761 1.389127

1 -9.846810 6.579826 2.559303

1 -8.945289 5.088679 2.254301

1 -8.095932 6.540025 2.804501

1 -10.864952 6.612625 0.297613

1 -9.887128 6.581846 -1.175623

1 -10.056075 5.118468 -0.196787

1 -6.810548 8.404874 -3.005775

1 -8.195052 8.210714 -1.928298

1 -6.628544 8.702036 -1.272734

1 -7.093263 6.078619 -3.926469

1 -7.085757 4.658460 -2.863586

1 -8.481848 5.740236 -2.888427

Compound **2**

6 2.232999 -2.396048 -0.000597

6 0.799935 -2.397425 -0.000605

6 0.088869 1.199719 -0.000335

6 0.799897 2.397394 -0.000253

6 2.232959 2.396039 -0.000268

6 2.942646 1.197742 -0.000352

6 0.831044 -0.000017 -0.000434

6 0.088885 -1.199762 -0.000509

6 -1.313730 -0.743295 -0.000435

6 -1.313737 0.743235 -0.000307

6 4.345392 -0.735351 -0.000371

6 2.942670 -1.197741 -0.000487

6 2.198801 -0.000006 -0.000431

6 4.345374 0.735381 -0.000380

7 -2.407447 -1.443303 -0.000420

6 -3.586365 -0.724637 -0.000261

6 -3.586370 0.724562 -0.000145

7 -2.407459 1.443235 -0.000189

7 5.447323 1.437394 -0.000305

6 6.612025 0.716175 -0.000240

6 6.612045 -0.716080 -0.000238

7 5.447362 -1.437334 -0.000305

6 -4.795772 -1.443124 -0.000177

6 -6.036499 -0.723437 0.000059

6 -6.036503 0.723349 0.000198

6 -4.795781 1.443043 0.000076

6 7.854531 1.426536 -0.000095

6 9.045949 0.700078 0.000010

6 9.045970 -0.699891 0.000027

6 7.854577 -1.426394 -0.000074

7 -7.186169 -1.418575 0.000170

6 -8.327997 -0.724614 0.000425

6 -8.328001 0.724515 0.000573

7 -7.186176 1.418481 0.000448

6 -9.577596 -1.419824 0.000547

6 -10.751028 -0.715786 0.000807

6 -10.751032 0.715675 0.000961

6 -9.577603 1.419719 0.000847

6 -4.800042 -2.860043 -0.000322

6 -4.800053 2.859962 0.000122

6 7.878592 -2.848615 0.000091

6 7.878456 2.848758 0.000007

6 -4.815291 -4.079973 -0.000440

6 7.947820 -4.066458 0.000408

6 7.947494 4.066612 0.000232

6 -4.815302 4.079891 0.000102

14 -4.848040 -5.899356 -0.000675

14 8.006141 -5.887267 0.001314

14 8.005236 5.887441 0.000558

14 -4.848037 5.899275 -0.000303

1 2.755457 -3.347975 -0.000662

1 0.278146 -3.349617 -0.000674

1 0.278090 3.349576 -0.000167

1 2.755406 3.347973 -0.000206

1 9.988563 1.237295 0.000113

1 9.988601 -1.237079 0.000146

1 -9.551093 -2.504810 0.000428

1 -11.701086 -1.242681 0.000902

1 -11.701092 1.242566 0.001173

1 -9.551105 2.504706 0.000963

1 -3.463006 -6.438470 -0.003748

1 -5.553287 -6.398887 1.208823

1 -5.558502 -6.398497 -1.207275

1 7.263796 -6.422670 -1.169460

1 7.388718 -6.417534 1.244773

1 9.416188 -6.350643 -0.070381

1 9.416882 6.351218 -0.013695

1 7.311792 6.420689 -1.200827

1 7.336693 6.419461 1.216528

1 -5.574356 6.398648 1.196701

1 -5.537251 6.398589 -1.219112

1 -3.463153 6.438364 0.020908

Compound **3**

6 -0.720709 -2.404193 0.019715

6 0.711074 -2.409789 0.009448

6 1.435909 1.185253 0.014952

6 0.729713 2.386592 0.020312

6 -0.702014 2.391982 0.027229

6 -1.417376 1.196186 0.029724

6 0.688985 -0.011569 0.017529

6 1.426787 -1.214047 0.007880

6 2.830623 -0.762445 -0.004172

6 2.836169 0.723152 0.004065

6 -2.827304 -0.740581 0.034384

6 -1.426991 -1.202960 0.027276

6 -0.679725 -0.006311 0.025843

6 -2.821171 0.745076 0.031809

7 3.922868 -1.465633 -0.023030

6 5.105333 -0.752756 -0.032153

6 5.110538 0.696973 -0.014411

7 3.933476 1.418513 0.001469

7 -3.912801 1.449213 0.027392

6 -5.095323 0.736675 0.028210

6 -5.101737 -0.712837 0.042830

7 -3.925048 -1.435352 0.042295

6 6.312613 -1.476998 -0.057976

6 7.554785 -0.758831 -0.066947

6 7.560136 0.688389 -0.041928

6 6.322509 1.413632 -0.011682

6 -6.301419 1.462722 0.011784

6 -7.545078 0.747234 0.021300

6 -7.551622 -0.700190 0.044404

6 -6.314689 -1.427605 0.054963

7 8.702498 -1.457233 -0.096811

6 9.846868 -0.767705 -0.101533

6 9.852859 0.680678 -0.075758

7 8.713600 1.378511 -0.046852

6 11.093522 -1.467734 -0.132816

6 12.270232 -0.769255 -0.137666

6 12.276176 0.661813 -0.112051

6 11.105737 1.370281 -0.082185

7 -8.692733 1.446769 0.008556

6 -9.838055 0.758478 0.018774

6 -9.844641 -0.690057 0.041051

7 -8.705785 -1.388932 0.053009

6 -11.084812 1.459014 0.007064

6 -12.261681 0.760793 0.016556

6 -12.268217 -0.670279 0.038112

6 -11.097773 -1.379168 0.049958

6 -6.325623 -2.843177 0.072078

6 -6.297566 2.878039 -0.017767

6 6.331494 2.828779 0.025859

6 6.312783 -2.892886 -0.074685

6 6.316556 -4.114791 -0.087300

6 -6.342533 -4.064776 0.084738

6 -6.299126 4.099367 -0.050923

6 6.346722 4.049713 0.069085

14 6.290193 -5.956391 -0.113303

14 -6.376483 -5.907257 0.058486

14 -6.307758 5.941817 -0.067256

14 6.364984 5.891663 0.114240

6 4.456955 -6.540991 -0.149664

6 7.296873 -6.518116 -1.652397

6 7.168037 -6.575234 1.477463

6 -4.776935 -6.466222 -0.842036

6 -7.926785 -6.416638 -0.947884

6 -6.572554 -6.490022 1.877902

6 -5.939063 6.545145 -1.855784

6 -8.025667 6.501762 0.568282

6 -4.920316 6.484143 1.140202

6 4.788956 6.460432 -0.818379

6 7.949178 6.460445 -0.798676

6 6.322588 6.466371 1.949775

6 3.849317 -6.669801 -1.559310

6 3.548788 -5.657952 0.731683

6 8.817875 -6.444226 -1.407337

6 6.947526 -5.726503 -2.929194

6 7.242872 -8.113801 1.542271

6 6.593458 -6.006278 2.787872

6 -4.592146 -7.995551 -0.882988

6 -3.498138 -5.767656 -0.338957

6 -7.841480 -5.983760 -2.423638

6 -9.218745 -5.874397 -0.304057

6 -5.374102 -6.139282 2.779406

6 -6.946961 -7.979044 2.017134

6 -6.423243 7.988069 -2.108099

6 -6.452500 5.601346 -2.960105

6 -8.229936 6.153007 2.055316

6 -9.176278 5.922516 -0.278777

6 -4.816962 8.010634 1.321650

6 -3.552306 5.879269 0.769550

6 4.637956 7.991635 -0.900198

6 3.510656 5.811035 -0.253446

6 7.893822 6.143590 -2.305873

6 9.224449 5.860352 -0.173351

6 6.887287 7.889382 2.140227

6 6.987702 5.484913 2.933705

1 -1.246434 -3.354388 0.019618

1 1.229085 -3.364131 0.003709

1 1.255456 3.336782 0.017535

1 -1.220709 3.346043 0.030624

1 11.061811 -2.552513 -0.151874

1 13.217843 -1.300104 -0.161284

1 13.228267 1.185109 -0.116756

1 11.085251 2.455356 -0.062690

1 -11.054374 2.543907 -0.009244

1 -13.209197 1.292264 0.007605

1 -13.220548 -1.193106 0.045009

1 -11.077192 -2.464292 0.066149

1 4.470334 -7.551152 0.290436

1 7.033659 -7.574298 -1.824483

1 8.195721 -6.194213 1.383669

1 -4.936279 -6.127058 -1.877173

1 -7.971920 -7.516924 -0.921714

1 -7.430595 -5.902308 2.239276

1 -4.839967 6.551675 -1.922281

1 -8.052040 7.598312 0.471972

1 -5.214024 6.053338 2.109224

1 4.920254 6.083054 -1.843558

1 7.998956 7.554654 -0.685744

1 5.251430 6.501725 2.203008

1 4.418629 -7.352251 -2.199882

1 3.800265 -5.697694 -2.064737

1 2.822161 -7.055804 -1.500082

1 3.535190 -4.622706 0.370599

1 3.875867 -5.630471 1.776073

1 2.517387 -6.038849 0.720867

1 9.145334 -7.091188 -0.586745

1 9.130595 -5.419290 -1.170776

1 9.367401 -6.752417 -2.307343

1 7.197569 -4.665899 -2.811054

1 5.886902 -5.787585 -3.189478

1 7.520442 -6.108000 -3.785582

1 7.837867 -8.439297 2.406484

1 6.246354 -8.559605 1.654527

1 7.700595 -8.551691 0.647163

1 7.225626 -6.286951 3.641592

1 6.527723 -4.913110 2.765851

1 5.589803 -6.398817 2.991265

1 -5.474069 -8.514419 -1.278038

1 -4.389960 -8.401073 0.115678

1 -3.739675 -8.268402 -1.519913

1 -3.238368 -6.084726 0.677794

1 -3.610087 -4.677726 -0.330202

1 -2.644941 -6.019031 -0.984993

1 -8.750168 -6.275642 -2.967764

1 -7.742228 -4.895024 -2.511898

1 -6.990214 -6.439103 -2.942277

1 -10.099970 -6.179291 -0.885389

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