Supporting Information:

Meta-analysis: the molecular organization of non-fullerene acceptors

Pierluigi Mondelli,[a] Gabriele Boschetto,[b] Peter N. Horton,[c] Priti Tiwana,[a] Chris-Kriton Skylaris,[b] Simon J. Coles,[c] Michal Krompiec[a] and Graham Morse[a]

[a] Merck Chemicals Ltd, Chilworth Technical Centre, University Parkway, Southampton SO16 7QD, UK. Email: graham.morse@merckgroup.com.
[b] School of Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ, UK.
[c] EPSRC Crystallographic Service, Department of Chemistry, University of Southampton, Highfield, SO17 1BJ, UK.

1. Crystallographic information

Table S1 Crystallographic information of the new crystal structures obtained in this work

Name	*ITIC*	*4TICO*	*m-4TICO*	*m-ITIC*
CCDC no.	1942946	1942947	1942948	1942949
Formula	$C_{94}H_{82}N_4O_2S_4$	$C_{104}H_{109}N_4O_8S_4$	$C_{100}H_{98}Cl_6N_4O_6S_4$	$C_{95}H_{83}Cl_3N_4O_2S_4$
$D_{calc.}$**/ g cm^{-3}**	1.255	1.238	1.322	1.261
μ**/mm^{-1}**	1.572	1.446	3.060	2.380
Formula Weight	1427.87	1671.19	1792.76	1547.24
Colour	metallic yellow	black	dark red	dark red
Shape	needle	rod	blade	needle
Size/mm^3	0.42×0.025×0.01	0.21×0.035×0.02	0.19×0.06×0.02	0.15×0.03×0.02
T**/K**	100(2)	100(2)	100(2)	100(2)
Crystal System	triclinic	monoclinic	triclinic	triclinic
Space Group	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
a**/Å**	14.9009(7)	15.2836(2)	8.6526(3)	8.7454(13)
b**/Å**	15.5043(4)	20.0101(5)	16.4878(8)	18.872(2)
c**/Å**	18.1199(5)	29.3242(6)	18.0435(8)	25.2647(18)
α**/°**	99.309(2)	90	114.697(5)	87.770(8)
β**/°**	101.541(3)	89.997(2)	103.822(4)	88.724(9)
γ**/°**	108.366(3)	90	90.890(4)	78.001(12)
V/Å^3	3777.2(2)	8968.1(3)	2251.45(19)	4075.1(9)
Z	2	4	1	2
Z'	1	1	0.5	1
Wavelength/Å	1.54178	1.54178	1.54178	1.54178
Radiation type	CuK_α	CuK_α	CuK_α	CuK_α
Θ_{min}**/°**	2.565	2.208	2.800	2.395
Θ_{max}**/°**	68.236	66.596	68.239	58.930
Measured Refl.	61232	62183	38283	43879
Independent Refl.	13714	15523	8194	11657
Reflections Used	8924	9046	6638	4311
R_{int}	0.1294	0.0953	0.0820	0.1316
Parameters	941	1174	627	1028
Restraints	0	2209	588	1813
Largest Peak	0.767	0.692	0.867	1.146
Deepest Hole	-0.570	-0.559	-0.667	-0.668
GooF	1.002	1.044	1.071	1.450

wR_2 (all data)	0.2080	0.2842	0.2158	0.5171
wR_2	0.1770	0.2395	0.2089	0.4418
R_1 (all data)	0.1126	0.1639	0.0852	0.3079
R_1	0.0718	0.0998	0.0753	0.1768

Name	*IEICO*	*IDIC*	*ICA*	*ICNA*	*IDT01*
CCDC no.	1942950	1942951	1942952	1942953	1942954
Formula	$C_{58}H_{60}Cl_3N_2O_2S_2$	$C_{66}H_{66}N_4O_2S_2$	$C_{23}H_{20}N_2OS$	$C_{27}H_{22}N_2OS$	$C_{20}H_{18}S_2$
$D_{calc.}$/ g cm^{-3}	1.260	1.240	1.325	1.346	1.300
μ/mm^{-1}	2.679	1.272	1.650	1.546	0.317
Formula Weight	987.55	1011.34	372.47	422.52	322.46
Colour	black	metallic yellow	red	dark red	Colourless
Shape	plate	plate	block	rod	block
Size/mm^3	0.36×0.18×0.015	0.10×0.06×0.02	0.28×0.22×0.08	0.22×0.04×0.03	0.20×0.20×0.16
T/K	100(2)	100(2)	100(2)	100(2)	120(2)
Crystal System	monoclinic	triclinic	triclinic	monoclinic	triclinic
Space Group	*C*2/*c*	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
a/Å	21.1745(9)	8.6679(4)	7.71450(10)	4.8299(2)	8.4290(2)
b/Å	35.242(2)	12.5073(7)	10.8650(2)	24.0080(5)	9.7140(3)
c/Å	14.1841(9)	13.5784(6)	12.5062(3)	17.9904(3)	11.0760(3)
α/°	90	72.096(4)	110.002(2)	90	82.096(2)
β/°	100.409(4)	75.545(4)	96.063(2)	91.295(2)	69.206(2)
γ/°	90	88.839(4)	104.290(2)	90	76.828(2)
V/Å^3	10410.5(10)	1353.88(12)	933.52(3)	2085.57(10)	823.92(4)
Z	8	1	2	4	2
Z'	1	0.5	1	1	1
Wavelength/Å	1.54178	1.54178	1.54178	1.54178	0.71073
Radiation type	CuK_a	CuK_a	CuK_a	CuK_a	MoK_a
Θ_{min}/°	3.699	3.538	3.846	3.070	3.066
Θ_{max}/°	68.235	68.242	68.234	68.233	27.603
Measured Refl.	28791	22142	16421	18627	19156
Independent Refl.	9244	4925	3390	3805	3772
Reflections Used	4070	4117	3349	3260	2914
R_{int}	0.1045	0.0496	0.0193	0.0428	0.0688
Parameters	716	336	245	301	203
Restraints	1314	0	0	3	0
Largest Peak	0.892	0.466	0.300	0.429	0.316
Deepest Hole	-0.602	-0.449	-0.289	-0.414	-0.392
GooF	1.470	1.056	1.047	1.081	1.055
wR_2 (all data)	0.4994	0.1508	0.0761	0.1478	0.1155
wR_2	0.4321	0.1441	0.0760	0.1424	0.1041
R_1 (all data)	0.2955	0.0640	0.0294	0.0611	0.0668
R_1	0.1903	0.0545	0.0292	0.0531	0.0466

2. Molecular considerations

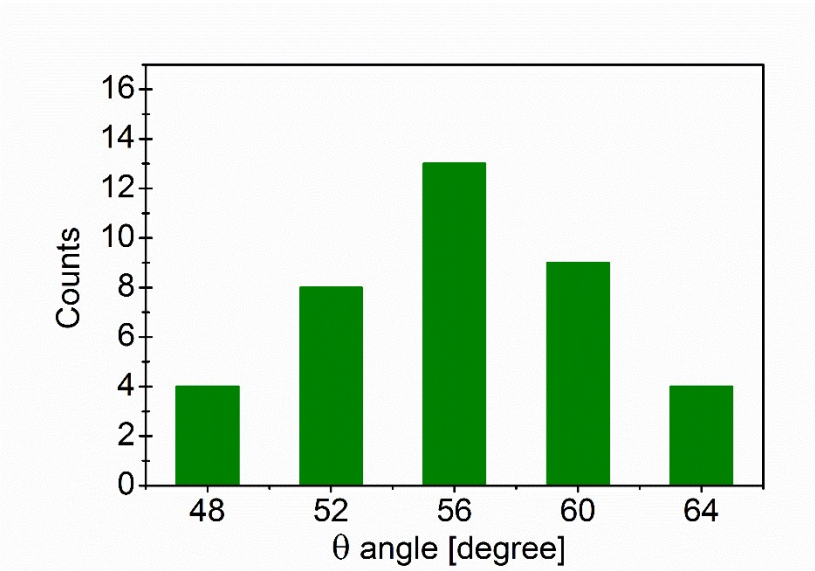

Figure S1 Distribution of the θ angle measured for the A-D-A family molecules

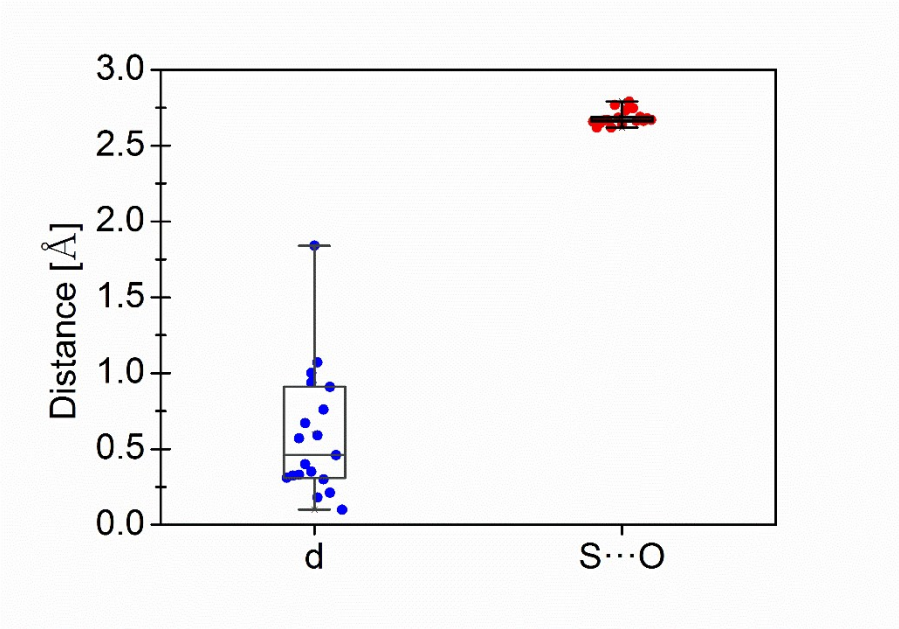

Figure S2 *d* distances and S···O close contacts measured for the A-D-A crystal structures studied in this work. The box plot denotes median (centre line), 25th (bottom edge of the box), 75th (top edge of the box), maximum and minimum values

3. Topological connectivity and charge transport

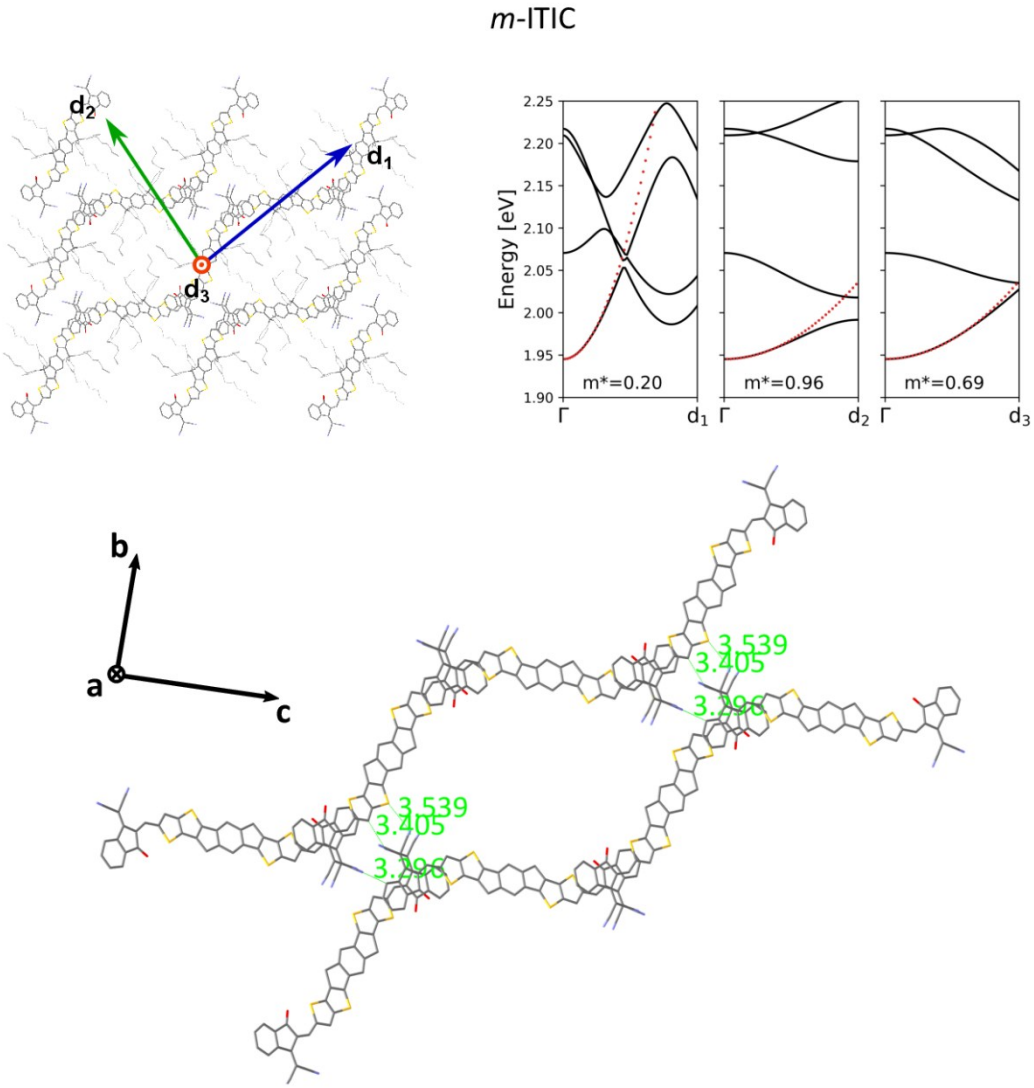

Figure S3 Top: View of the brickwork 2D packing motif of *m*-ITIC with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Bottom: shortest close contacts between non-interconnected molecules are drawn in green. Sidechains, solvent inclusions and hydrogen atoms have been omitted for clarity.

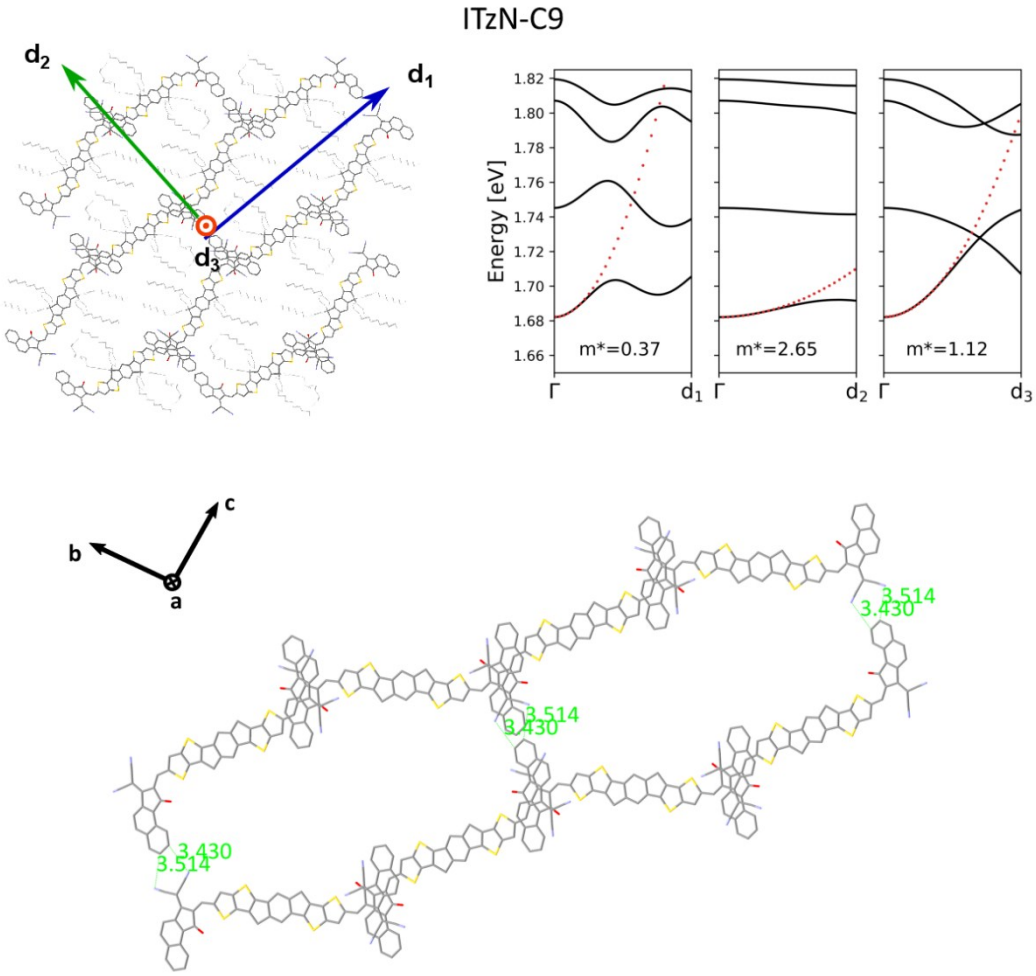

Figure S4 Top: View of the brickwork 2D packing motif of ITzN-C9 with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Bottom: shortest close contacts between non-interconnected molecules are drawn in green. Sidechains, solvent inclusions and hydrogen atoms have been omitted for clarity.

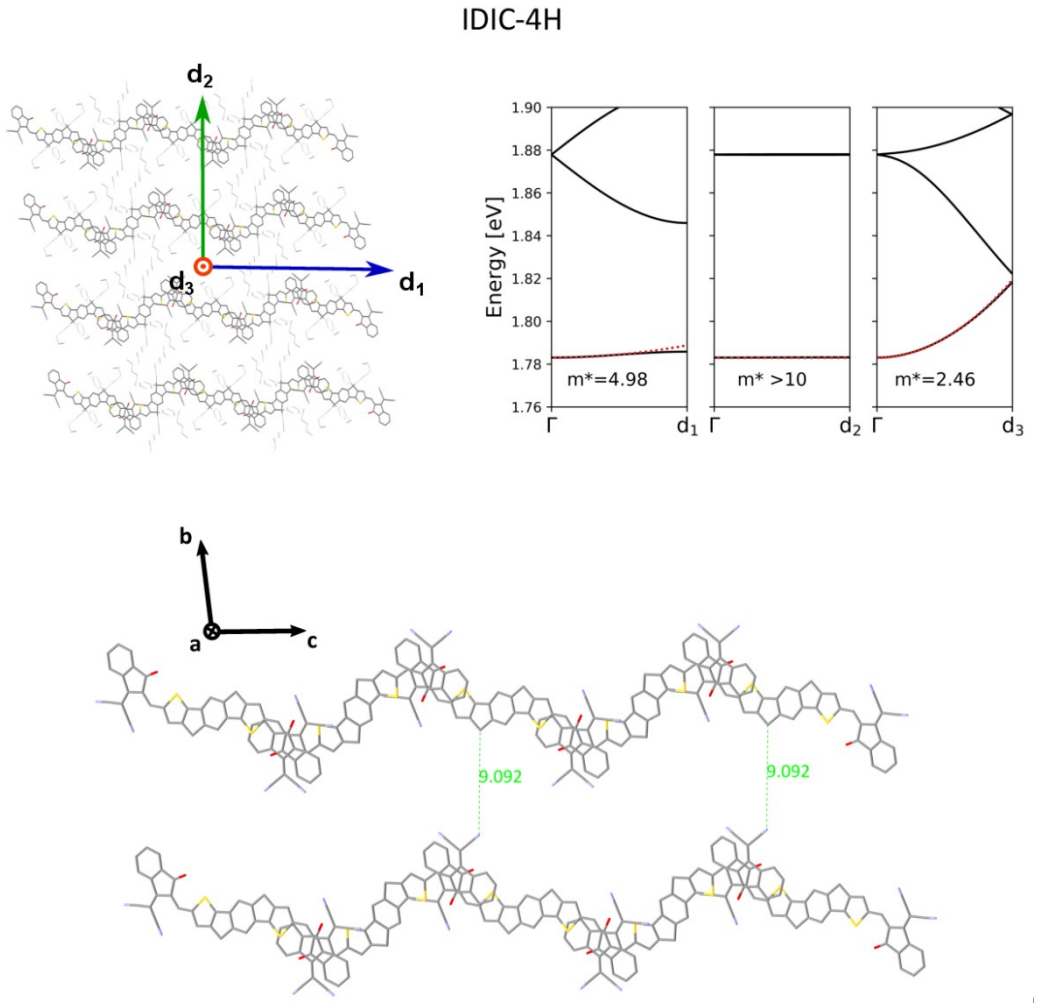

Figure S5 Top: view of the brickwork 2D packing motif of IDIC-4H with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown . Bottom: shortest distances between non-interconnected molecules are drawn in green. Sidechains and hydrogen atoms have been omitted for clarity.

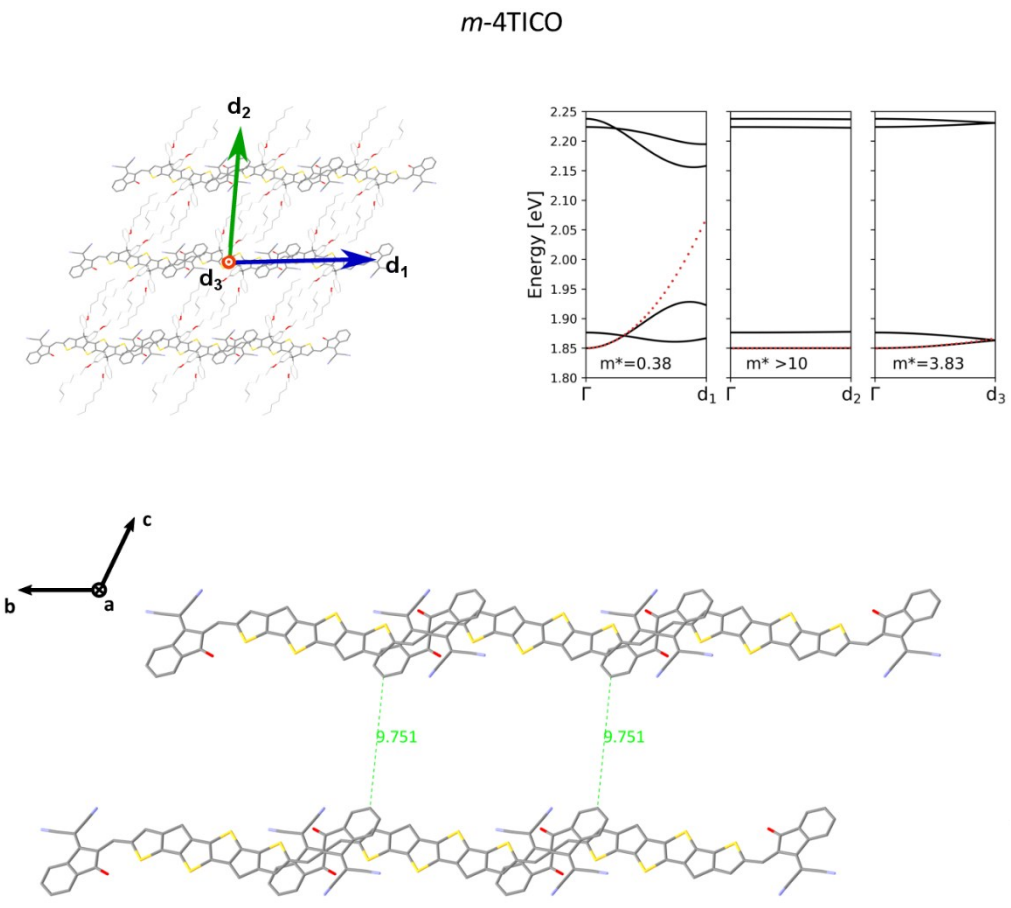

Figure S6 Top: view of the brickwork 2D packing motif of *m*-4TICO with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Bottom: shortest distances between non-interconnected molecules are drawn in green. Sidechains, solvent inclusions and hydrogen atoms have been omitted for clarity.

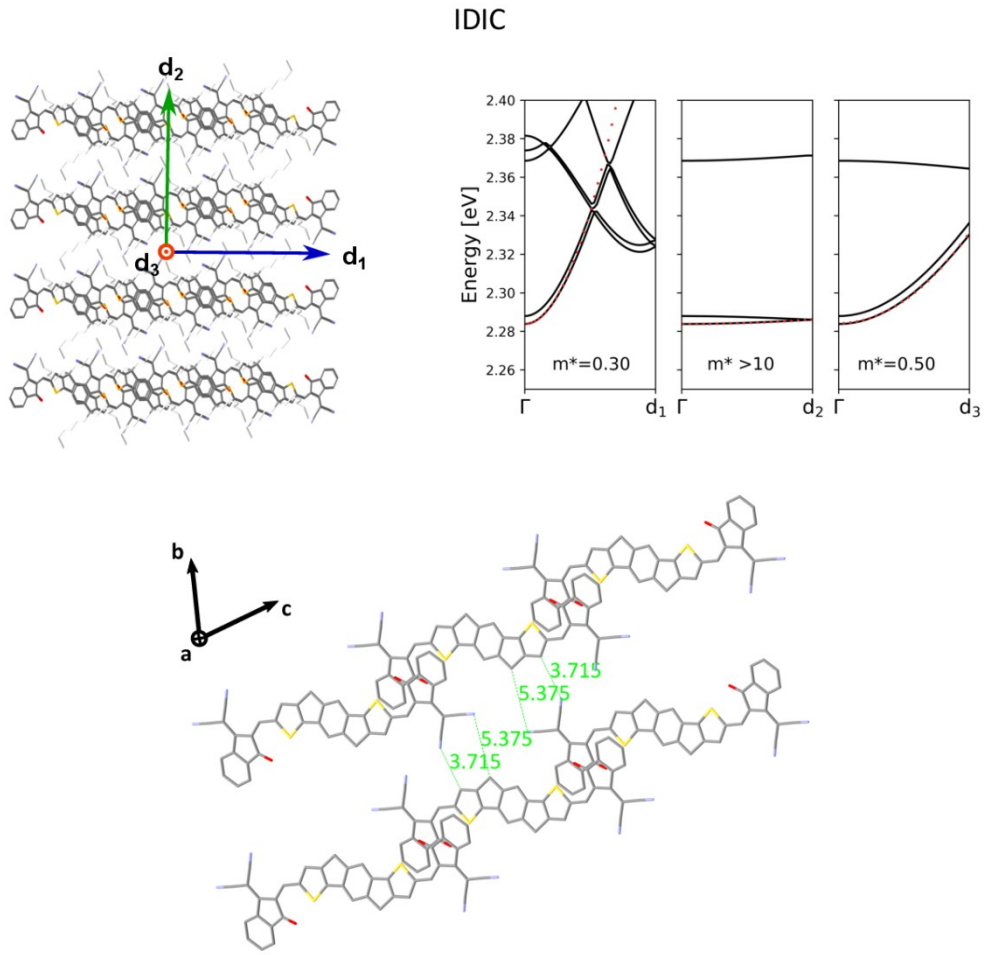

Figure S7 Top: view of the brickwork 2D packing motif of IDIC with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Bottom: shortest distances between non-interconnected molecules are drawn in green (Bottom). Sidechains and hydrogen atoms have been omitted for clarity.

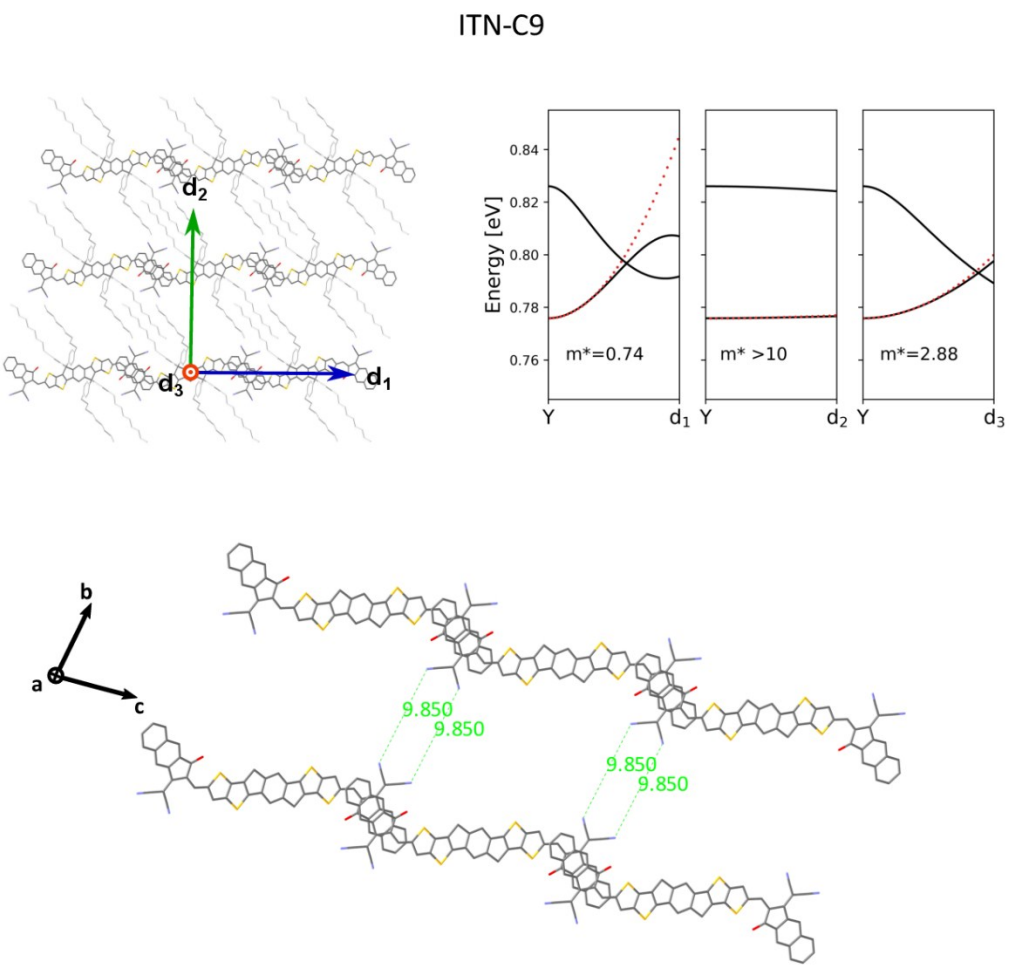

Figure S8 Top: view of the brickwork 2D packing motif of ITN-C9 with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Bottom: shortest distances between non-interconnected molecules are drawn in green (Bottom). Sidechains, solvent inclusions and hydrogen atoms have been omitted for clarity.

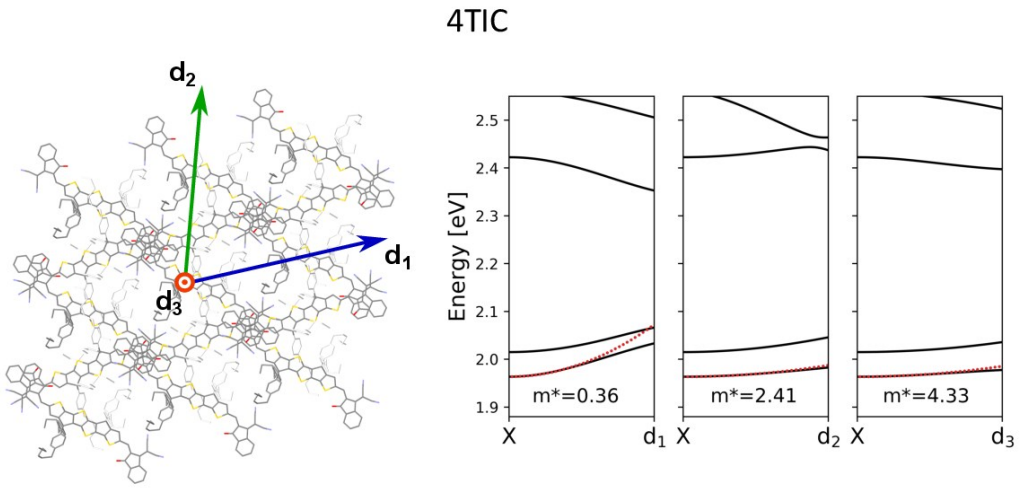

Figure S9 Top view of the reticular 3D packing motif of 4TIC with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Solvent inclusions and hydrogen atoms have been omitted for clarity.

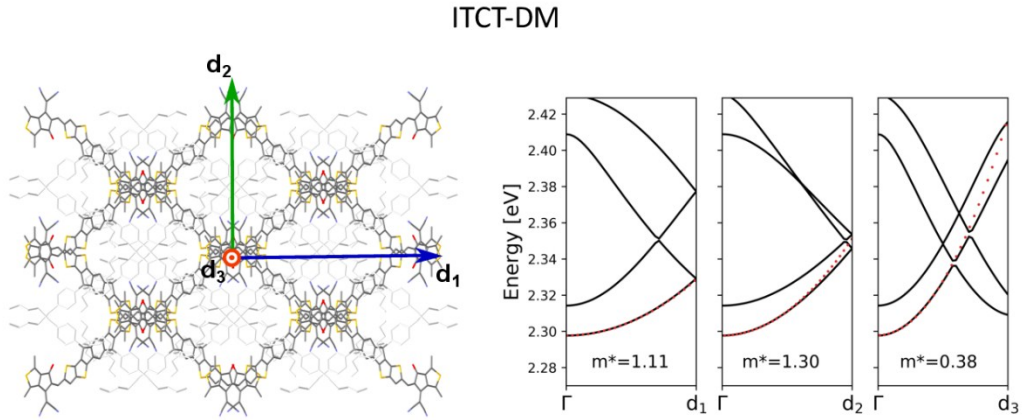

Figure S10 Top view of the reticular 3D packing motif of ITCT-DM with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Hydrogen atoms have been omitted for clarity.

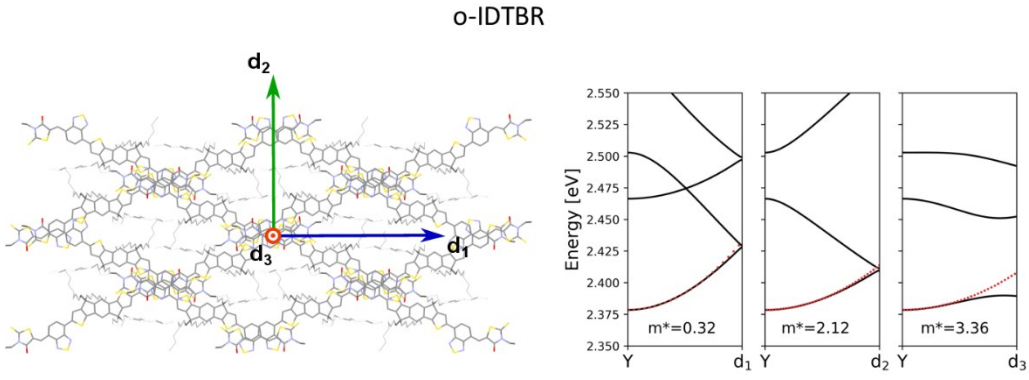

Figure S11 Top view of the reticular 3D packing motif of *o*-IDTBR with d_1, d_2 and d_3 directions superimposed. Calculated conduction band along d_1, d_2 and d_3 directions and effective mass are shown. Hydrogen atoms have been omitted for clarity.