

Chapter 1

Material Properties

Common Name	Chemical Name	Other Names	HOMO	LUMO	E _T	CAS	T _{melt}	M.W.	τ
3TPYMB	b'Tris(2,4,6-triMethyl-3-(pyridin-3-yl)phenyl)borane'		6.7	3.3		929203021		599.61	
4CzIPN	b'(4s,6s)-2,4,5,6-tetra(9H-carbazol-9-yl)isophthalonitrile'		5.8	3.4		1416881521		788.89348	
Ag	b'Silver'	silver ag	4.6	4.6		7440224	962.0	107.868	
Air									
Al	b'Aluminum'			4.3		7429905	660.0	26.981	
Alq3	b'Tris(8-hydroxyquinoline)aluminum'	Tris(8-hydroxyquinolato)aluminum	5.62	2.85		2085338		459.43	
		Aluminum oxinate							
		Aluminum 8-hydroxyquinolate							
		8-Hydroxyquinoline aluminum salt							
Anthracene	b'Anthracene'		5.7	1.7		120127		178.23	
AQ1200	b''			5.5					
AQ1250				5.5					
Au	b'Gold'	gold au	5.1	5.1		7440575	1064.0	196.97	

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B3PYMPM	b'bis-4,6-(3,5-di-3-pyridylphenyl)-2-methylpyrimidine'		6.8	3.3		925425963		554.64	
BCBP	b"2,2'-Bis(4-(carbazol-9-yl)phenyl)-biphenyl"		6.1	2.6		858131701		636.78	
BCP	b'Bathocuproine'		6.5 7.0	1.6 3.5		4733395		360.45	
BP2T	b'5,5u-[Di(1,1u-biphenyl)-4-yl]-2,2u-bithiophene'		5.3	2.8		175850289		470.658	
BP4mPy	b'3,5,3A,5A-tetra(m-pyrid-3-yl)phenyl[1,1']biphenyl'biphenyl'	3,5,3',5'-tetra(m-pyrid-3-yl)phenyl[1,1']biphenyl	6.66	2.57		1009033946	191	766.93	
Bphen	b'Bathophenanthroline'	4,7-Diphenyl-1,10-phenanthroline	6.4	3.0		1662017		332.4	
BPy-TP2	b'2,7-Bis(2,20-bipyridine-5-yl)triphenylene'		5.7	2.7		1394813581		536.624	
c-TiO2									
C60	b'Fullerene'	fullerene	6.1	3.7 3.5		99685968		720.64	
C70	b'[5,6]-Fullerene'	fullerene C60	6.3			115383227		840.75	

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CBP	b'4,4-Bis(N-carbazolyl)-1,1-biphenyl'		6.1	1.9		58328317		484.59	0.7
CDBP	b"4,4'-Bis(9-carbazolyl)-2,2'-dimethylbiphenyl"		6.0	2.9		120260017		512.64	
ClAlPc	b'Aluminum phthalocyanine chloride'					14154428		574.96	
CuPc	b'Copper(II) phthalocyanine'		4.8	2.6		147148		576.07	
CzSi	b'9-(4-tert-butylphenyl)-3,6-bis(triphenylsilyl)-9H-carbazole'		5.2	3.5					
			6.0	2.5		898546822		816.19	
CzTRZ	b'9-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]-9H-carbazole'		6.08	3.28		nan		nan	
Dow ETL			5.1	1.808					
Dow ETL2			5.842	1.908					
Dow HIL			4.509	1.128					
Dow Host A			5.669	2.269					

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				1.223					
Dow Host B			5.261	2.361 1.872					
Dow HTL			4.736	1.039					
DPDCPB	b'2-[7-(4-Diphenylaminophenyl)-2,1,3-benzothiadiazol-4-yl]methylenepropanedinitrile'		5.5	3.36		1393343606		455.53	
DPDCTB	b''		5.35	3.44					
DTDCPB	b'2-[(7-4-[N,N-Bis(4-methylphenyl)amino]phenyl)-2,1,3-benzothiadiazol-4-yl]methylenepropanedinitrile'		5.43	3.35		1393343582		483.59	
DTDCTB	b'2-[7-(5-N,N-Ditolylaminothiophen-2-yl)-2,1,3-benzothiadiazol-4-yl]methylenemalononitrile'		5.3	3.44		1335150098		489.61	
Flrpic	b'Bis[2-(4,6-difluorophenyl)pyridinato-C2,N](picolinato)iridium(III)'		5.8	2.9		376367930		694.66	
Glass	b'Silicon Dioxide'								

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H2Pc	b'29H,31H- Phthalocyanine'					574936		514.54	
HATCN	b'1,4,5,8,9,11- Hexaazatriphenylenhexacarbonitrile'		9.5 7.5	5.5 4.4		105598274		384.27	
Hoye CoOMe									
Hoye Nap CoOMe									
Hoye Nap NPh2									
Hoye Nap OMe									
Hoye Nap H									
Hoye OH									
Hoye OMe									
Hoye Triben-H									
Hoye Triben OMe									
Hoye OMe	b''		6.07	2.55					
Ir(dpm)PQ2	b'Bis(2- phenylquinoline)(2,2,6,6- tetramethylheptane- 3,5- dionate)iridium(III)'					713079039		783.98	
Ir(mphq)3	b'Tris[2-phenyl-4- methylquinoline]iridium(III)'					1433853907		847.04	

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Ir(ppy) ₃	b'Tris[2-phenylpyridinato-C ₂ N]iridium(III)'		5.1	2.6		94928866		654.78	1000.0
ITO	b'Indium Tin Oxide'					50926119			
Li(acac)									
LiF	b'Lithium Fluoride'			2.8		7789244		25.94	
LiQ	b'8-Quinololato lithium (Liq)'		4.667	1.292		25387933		151.09	
MADN	b'2-Methyl-9,10-bis(naphthalen-2-yl)anthracene'		5.6	2.6		804560007		444.57	
MAI									
mCBP	b"3,3'-Bis(N-carbazolyl)-1,1'-biphenyl"		6.0	2.4		342638544		484.58916	
mCP	b'1,3-Bis(N-carbazolyl)benzene'		6.1 5.9	2.4		550378784	187.0	408.49	
MgPc	b'Magnesium phthalocyanine'					1661036		536.83	
MoOx	b'Molybdenum(VI) oxide'					1313275		143.94	

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NPD	b'N,N-Di(1-naphthyl)- N,N-diphenyl-(1,1- biphenyl)-4,4-diamine'		5.3 5.4 5.4	2.3 1.52 2.4		123847858	280.0	588.74	3.5
NTCDA	b'1,4,5,8- Naphthalenetetracarboxylic dianhydride'		7.9	4.0		81301		268.18	
NTU1	b'2-[7-(4-ethyl-4H- thieno[3,2-b]indol-2- yl)benzo[c][1,2,5]thiadiazol- 4-yl]- methylenemalononitrile'								
NTU2	b'2-[7-(8-ethyl- 8Hthieno[2,3-b]indol-2- yl)benzo[c][1,2,5]thiadiazol- 4-yl]- methylenemalononitrile'								
P3HT	b'Poly(3- hexylthiophene-2,5- diyl)'					156074985			
PbPc	b'Lead(II) phthalocya- nine'					15187163		719.72	

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Pedot	b'Poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate)'								
Pentacene	b'Pentacene'		5.2 4.85 5.0	3.0 2.8 3.2		135488	300.0	278.35	
Perfluoropentacene	b'perfluoropentacene'		6.7	5.0		646533882		530.22	
PO-T2T	b'2,4,6-Tris[3-(diphenylphosphinyl)phenyl]-1,3,5-triazine'		6.83 7.5	2.83 3.5		1646906264	287	909.8	
PPT	b'2,8-Bis(diphenylphosphoryl)dibenzo[b,d]thiophene'					1019842999		584.6	
PQIr	b'(2,4-Pentanedionato)bis[2-(2-quinoliny)phenyl]iridium(III)'					337526951		699.82	
Pt17									
PTCBI	b'3,4,9,10-Perylenetetracarboxylic Bisbenzimidazole '		6.2	4.3		79534911		536.54	
PTCDA	b'Perylene-3,4,9,10-tetracarboxylic dianhydride'		6.95	4.1		128698		392.32	3.2

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PTCDI	b'N,N-Dioctyl-3,4,9,10- perylene dicarboximide'	PTCDI-C8	6.2	6.2		78151583		614.77	
PtOEP	b'Platinum octaethyl- porphyrin'					31248392		727.84	
PtTPBP	b'Platinum(II) tetraphenyltetra- benzoporphyrin'	[6,13,20,27- Tetraphenyl-29H,31H- tetrabenzoporphinato(2-)- κ 2N29,N31]platinum Pt(II) meso- Tetraphenyl Tetra- benzoporphine platinum tetraphenyl- tetrabenzoporphine PtTPBP	4.8	2.9		166174056		1008.0	
Quartz									
Rubrene	b'5,6,11,12- Tetraphenyl naphthacene'		4.85	3.15		517511		532.67	9.1
			5.3	2.7					
			4.47	1.88					
			4.45	1.88					
			4.51	1.95					
			4.83	2.18					
			4.85	2.2					
			4.92	2.27					

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SnI22									
SnNcCl2	b'Tin(IV) 2,3-naphthalocyanine dichloride'					26857614		902.37	
SubNc	b'Boron sub-2,3-naphthalocyanine chloride'	SubNc-Cl	5.35	3.47		142710563		580.83	
SubPc	b'Boron subphthalocyanine chloride'	SubPc-Cl	5.5	3.5					
			5.6	3.2		36530060	375.0	430.66	0.5
T2T	b'2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine'		5.57	3.6					
			6.5	3.0		1201800830		537.652	
TAPC	b'4,4-Cyclohexylidenebis[N,N-bis(4-methylphenyl)benzenamine]'		5.5	1.8		58473782		626.87	
TAZ	b'3-(Biphenyl-4-yl)-5-(4-tert-butylphenyl)-4-phenyl-4H-1,2,4-triazole'		6.3	2.7		150405699		429.56	
TCCTA	b'Tris(4-carbazoyl-9-ylphenyl)amine'		5.7	2.4		139092787		740.89	
Tetracene	b'Benz[b]anthracene'		5.1	1.8		92240		228.29	

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TmPyPB	b'1,3,5-Tri(m-pyrid-3-ylphenyl)benzene'		6.63	2.54		921205030	181	537.65	
TPBi	b'2,2,2"-(1,3,5-Benzinetriyl)-tris(1-phenyl-1-H-benzimidazole)'		6.1	2.8		192198859		654.76	
TPD	b'N,N-Bis(3-methylphenyl)-N,N-diphenylbenzidine'		5.5	2.3		65181784		516.67	
Tris-PCz	b'9,9,9-triphenyl-9H,9H,9H-3,3,6,3-tercarbazole'	9,9'-Diphenyl-6-(9-phenyl-9H-carbazol-3-yl)-9H,9'H-3,3'-bicarbazole	5.6	2.1		1141757836		725.88	
UGH2	b'p-Bis(triphenylsilyl)benzene;Benzene,1,4-bis(triphenylsilyl)-;1,4-Phenylenebis(triphenylsilane);1,4-Phenylenebis(triphenylsilane)'		7.2	2.8		18856081	345.0	594.89	
ZnPc	b'Zinc phthalocyanine'		5.28	3.3		14320048		577.91	