Mei-Yin Chou

List of Publications by Year in Descending Order

164 papers	12,555 citations	54 h-index	110 g-index
171 ext. papers	13,859 ext. citations	6 avg, IF	6.27 L-index

#	Paper	IF	Citations
164	Structure Relaxation and Liquidlike Enhanced Cu Diffusion at the Surface of CuS Chalcocite. *Nano Letters*, **2021**, 21, 8895-8900	11.5	0
163	Embedment of Multiple Transition Metal Impurities into WS Monolayer for Bandstructure Modulation. *Small*, **2021**, 17, e2007171	11	0
162	Epitaxial Growth of Two-Dimensional Insulator Monolayer Honeycomb BeO. *ACS Nano*, **2021**, 15, 2497-2505	16.7	13
161	Coherent Electronic Band Structure of TiTe/TiSe Moir Bilayer. *ACS Nano*, **2021**, 15, 3359-3364	16.7	1
160	Mechanism for anisotropic diffusion of liquid-like Cu atoms in hexagonal u2S. *Physical Review Materials*, **2021**, 5,	3.2	1
159	Critical role of parallel momentum in quantum well state couplings in multi-stacked nanofilms: An angle resolved photoemission study. *AIP Advances*, **2020**, 10, 125211	1.5	
158	Liquidlike Cu atom diffusion in weakly ionic compounds Cu2S and Cu2Se. *Physical Review B*, **2020**, 102,	3.3	8
157	End-Bonded Metal Contacts on WSe Field-Effect Transistors. *ACS Nano*, **2019**, 13, 8146-8154	16.7	30
156	Theoretical study of quantum size effects in thin Al(100), Al(110), and Al(111) films. *Physical Review B*, **2019**, 99,	3.3	5
155	Thermoelectric Figure-of-Merit of Fully Dense Single-Crystalline SnSe. *ACS Omega*, **2019**, 4, 5442-5450	3.9	28
154	Ultrafast Monolayer In/Gr-WS-Gr Hybrid Photodetectors with High Gain. *ACS Nano*, **2019**, 13, 3269-3279	16.7	26
153	Origin of Band Modulation in GeTe-Rich GeSbTe Thin Film. *ACS Applied Electronic Materials*, **2019**, 1, 2619-2625	4	2
152	Gapped electronic structure of epitaxial stanene on InSb(111). *Physical Review B*, **2018**, 97,	3.3	68
151	Tuning Band Gap and Work Function Modulations in Monolayer hBN/Cu(111) Heterostructures with Moir Patterns. *ACS Nano*, **2018**, 12, 9355-9362	16.7	19
150	In Situ Strain Tuning of the Dirac Surface States in BiSe Films. *Nano Letters*, **2018**, 18, 5628-5632	11.5	17
149	Electrical valley filtering in transition metal dichalcogenides. *Physical Review Materials*, **2018**, 2,	3.2	9
148	Unique Gap Structure and Symmetry of the Charge Density Wave in Single-Layer VSe_{2}. *Physical Review Letters*, **2018**, 121, 196402	7.4	90

147	Stable 1T Tungsten Disulfide Monolayer and Its Junctions: Growth and Atomic Structures. *ACS Nano*, **2018**, 12, 12080-12088	16.7	51
146	Topological Properties of Gapped Graphene Nanoribbons with Spatial Symmetries. *Nano Letters*, **2018**, 18, 7254-7260	11.5	12
145	Large quantum-spin-Hall gap in single-layer 1TNWSe. *Nature Communications*, **2018**, 9, 2003	17.4	74
144	Interlayer couplings, Moir patterns, and 2D electronic superlattices in MoS/WSe hetero-bilayers. *Science Advances*, **2017**, 3, e1601459	14.3	277
143	Janus monolayers of transition metal dichalcogenides. *Nature Nanotechnology*, **2017**, 12, 744-749	28.7	828
142	Tailoring Semiconductor Lateral Multijunctions for Giant Photoconductivity Enhancement. *Advanced Materials*, **2017**, 29, 1703680	24	17
141	Emergence of charge density waves and a pseudogap in single-layer TiTe. *Nature Communications*, **2017**, 8, 516	17.4	63
140	Ultrahigh thermoelectric performance in Cu2Se-based hybrid materials with highly dispersed molecular CNTs. *Energy and Environmental Science*, **2017**, 10, 1928-1935	35.4	215
139	Elemental Topological Dirac Semimetal: Sn on InSb(111). *Physical Review Letters*, **2017**, 118, 146402	7.4	71
138	Strain Engineering a 4 Charge Density Wave Phase in Transition Metal Dichalcogenide 1T-VSe. *Physical Review Materials*, **2017**, 1,	3.2	32
137	Dimensional Effects on the Charge Density Waves in Ultrathin Films of TiSe. *Nano Letters*, **2016**, 16, 6331-6336	11.5	46
136	Ca3P2 and other topological semimetals with line nodes and drumhead surface states. *Physical Review B*, **2016**, 93,	3.3	230
135	Spin texture in type-II Weyl semimetal WTe2. *Physical Review B*, **2016**, 94,	3.3	83
134	Hidden Order and Dimensional Crossover of the Charge Density Waves in TiSe. *Scientific Reports*, **2016**, 6, 37910	4.9	24
133	Bandgap renormalization and work function tuning in MoSe/hBN/Ru(0001) heterostructures. *Nature Communications*, **2016**, 7, 13843	17.4	51
132	Theory of valley-dependent transport in graphene-based lateral quantum structures. *Physical Review B*, **2016**, 94,	3.3	9
131	Determination of band alignment in the single-layer MoS2/WSe2 heterojunction. *Nature Communications*, **2015**, 6, 7666	17.4	421
130	Strong Asymmetric Charge Carrier Dependence in Inelastic Electron Tunneling Spectroscopy of Graphene Phonons. *Physical Review Letters*, **2015**, 114, 245502	7.4	37

129	Charge density wave transition in single-layer titanium diselenide. *Nature Communications*, **2015**, 6, 8943	17.4	154
128	Ultrahigh-gain photodetectors based on atomically thin graphene-MoS2 heterostructures. *Scientific Reports*, **2014**, 4, 3826	4.9	678
127	Ultrafast Bulk Diffusion of AlHx in High-Entropy Dehydrogenation Intermediates of NaAlH4. *Journal of Physical Chemistry C*, **2014**, 118, 18356-18361	3.8	3
126	Pressure-induced antiferrodistortive phase transition in SrTiO 3 : Common scaling of soft-mode with pressure and temperature. *Europhysics Letters*, **2014**, 107, 36006	1.6	9
125	Electron-phonon coupling in two-dimensional silicene and germanene. *Physical Review B*, **2013**, 88,	3.3	92
124	Coupled Dirac fermions and neutrino-like oscillations in twisted bilayer graphene. *Nano Letters*, **2013**, 13, 5159-64	11.5	14
123	Stability and electronic properties of two-dimensional silicene and germanene on graphene. *Physical Review B*, **2013**, 88,	3.3	153
122	Surface passivation and orientation dependence in the electronic properties of silicon nanowires. *Journal of Physics Condensed Matter*, **2013**, 25, 145501	1.8	13
121	Magnetic-field dependence of low-lying spectra in bilayer graphene-based magnetic dots and rings. *Solid State Communications*, **2013**, 156, 49-53	1.6	3
120	Anomalous phase relations of quantum size effects in ultrathin Pb films on Si(111). *Physical Review B*, **2013**, 87,	3.3	10
119	Hydrogen Interaction with the Al Surface Promoted by Subsurface Alloying with Transition Metals. *Journal of Physical Chemistry C*, **2012**, 116, 18663-18668	3.8	18
118	Fractal Landau-level spectra in twisted bilayer graphene. *Nano Letters*, **2012**, 12, 3833-8	11.5	70
117	Quantum Monte Carlo investigations of adsorption energetics on graphene. *Journal of Physics Condensed Matter*, **2012**, 24, 395002	1.8	7
116	Charge transport through graphene junctions with wetting metal leads. *Nano Letters*, **2012**, 12, 3424-30	11.5	16
115	Diffusion of Si and C atoms on and between graphene layers. *Journal Physics D: Applied Physics*, **2012**, 45, 455309	3	16
114	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. *Physical Review B*, **2012**, 85,	3.3	15
113	Optical phonon anomaly in Bernal stacked bilayer graphene with ultrahigh carrier densities. *Physical Review B*, **2012**, 86,	3.3	3
112	Lattice vibrational modes and their frequency shifts in semiconductor nanowires. *Nano Letters*, **2011**, 11, 2618-21	11.5	17

111	Theoretical study of the vibrational properties of NaAlH4 with AlH3 vacancies. *Faraday Discussions*, **2011**, 151, 243-51; discussion 285-95	3.6	2
110	Stability of the hydrogen-storage compound Li6Mg(NH)4 from first principles. *Physical Review B*, **2011**, 83,	3.3	2
109	Effects of electrostatic fields and charge doping on the linear bands in twisted graphene bilayers. *Physical Review B*, **2011**, 84,	3.3	32
108	Catalytic effect of near-surface alloying on hydrogen interaction on the aluminum surface. *Physical Review B*, **2011**, 83,	3.3	17
107	Enhanced optical conductivity induced by surface states in ABC-stacked few-layer graphene. *Physical Review B*, **2011**, 83,	3.3	16
106	Quantum size effects on the work function of metallic thin film nanostructures. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 12761-5	11.5	54
105	Theoretical investigation of intermediate phases between Li2NH and LiNH2. *Physical Review B*, **2010**, 82,	3.3	5
104	Effects of metallic contacts on electron transport through graphene. *Physical Review Letters*, **2010**, 104, 076807	7.4	130
103	Low-lying spectra of massless Dirac electron in magnetic dot and ring. *Applied Physics Letters*, **2010**, 96, 212101	3.4	12
102	Energy spectra of a single-electron magnetic dot using the massless Dirac-Weyl equation. *Journal of Physics Condensed Matter*, **2010**, 22, 355501	1.8	3
101	Oxidation functional groups on graphene: Structural and electronic properties. *Physical Review B*, **2010**, 82,	3.3	272
100	Path to Wigner localization in circular quantum dots. *Physical Review B*, **2009**, 79,	3.3	13
99	Phase relations associated with one-dimensional shell effects in thin metal films. *Physical Review Letters*, **2009**, 102, 236803	7.4	37
98	First-principles investigation of sodium and lithium alloyed alanates. *Journal of Alloys and Compounds*, **2009**, 479, 678-683	5.7	9
97	Structural and electronic properties of oxidized graphene. *Physical Review Letters*, **2009**, 103, 086802	7.4	408
96	Electron-phonon interactions for optical-phonon modes in few-layer graphene: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	38
95	Quantum confinement effect in Si/Ge core-shell nanowires: First-principles calculations. *Physical Review B*, **2008**, 77,	3.3	64
94	Size- and Strain-Dependent Electronic Structures in H-Passivated Si [112] Nanowires. *Journal of Physical Chemistry C*, **2008**, 112, 15680-15683	3.8	24

93	Alanates as hydrogen storage materials **2008**, 381-419		3
92	Electronic and vibrational properties of □AlH3. *Physical Review B*, **2008**, 77,	3.3	23
91	Low-energy ordered structures of Li2Mg(NH)2. *Journal of Applied Physics*, **2008**, 104, 083519	2.5	9
90	Phonon dispersions and vibrational properties of monolayer, bilayer, and trilayer graphene: Density-functional perturbation theory. *Physical Review B*, **2008**, 77,	3.3	170
89	First-principles study of cation and hydrogen arrangements in the Li-Mg-N-H hydrogen storage system. *Physical Review B*, **2007**, 76,	3.3	22
88	Quantum size effect in Pb(100) films: Critical role of crystal band structure. *Physical Review B*, **2007**, 75,	3.3	21
87	LaMg2PdH7, a new complex metal hydride containing tetrahedral [PdH4]4□anions. *Journal of Alloys and Compounds*, **2007**, 446-447, 34-38	5.7	11
86	Size and orientation dependence in the electronic properties of silicon nanowires. *Physical Review B* , **2007**, 76,	3.3	93
85	Enhanced electron-hole interaction and optical absorption in a silicon nanowire. *Physical Review B*, **2007**, 75,	3.3	57
84	Lattice dynamics and thermodynamic properties of NaAlH4: Density-functional calculations using a linear response theory. *Physical Review B*, **2006**, 73,	3.3	17
83	Exchange-correlation energy in molecules: A variational quantum Monte Carlo study. *Physical Review A*, **2006**, 74,	2.6	6
82	Beyond the local approximation to exchange and correlation: The role of the Laplacian of the density in the energy density of Si. *Physical Review B*, **2006**, 74,	3.3	17
81	Persistent superconductivity in ultrathin Pb films: a scanning tunneling spectroscopy study. *Physical Review Letters*, **2006**, 96, 027005	7.4	232
80	Zhao et al. Reply:. *Physical Review Letters*, **2005**, 94,	7.4	7
79	Hydrogenation-induced insulating state in the intermetallic compound LaMg2Ni. *Physical Review Letters*, **2005**, 94, 066403	7.4	34
78	First-principles study of NaAlH4 and Na3AlH6 complex hydrides. *Physical Review B*, **2004**, 70,	3.3	78
77	Thermal stability and electronic structure of atomically uniform Pb films on Si(111). *Physical Review Letters*, **2004**, 93, 026802	7.4	143
76	Alternative low-symmetry structure for 13-atom metal clusters. *Physical Review Letters*, **2004**, 93, 133401	7.4	181

75	Quantum confinement and electronic properties of silicon nanowires. *Physical Review Letters*, **2004**, 92, 236805	7.4	438
74	First-principles studies of quasiparticle band structures of cubic YH3 and LaH3. *Physical Review B*, **2003**, 67,	3.3	28
73	Alternating layer and island growth of Pb on Si by spontaneous quantum phase separation. *Physical Review Letters*, **2003**, 90, 076104	7.4	78
72	Effects of the substrate on quantum well states: A first-principles study for Ag/Fe(100). *Physical Review B*, **2003**, 68,	3.3	34
71	Electron-hole coupling and the charge density wave transition in TiSe2. *Physical Review Letters*, **2002**, 88, 226402	7.4	161
70	Kidd et al. Reply:. *Physical Review Letters*, **2002**, 88,	7.4	7
69	Fermi surfaces and energy gaps in Sn/Ge(111). *Journal of Physics Condensed Matter*, **2002**, 14, R1-R20	1.8	37
68	Atomic-layer-resolved quantum oscillations in the work function: Theory and experiment for Ag/Fe(100). *Physical Review B*, **2002**, 66,	3.3	82
67	Theory of quantum size effects in thin Pb(111) films. *Physical Review B*, **2002**, 66,	3.3	244
66	X-ray studies of phonon softening in tise2. *Physical Review Letters*, **2001**, 86, 3799-802	7.4	110
65	Comparative study of density-functional theories of the exchange-correlation hole and energy in silicon. *Physical Review B*, **2001**, 64,	3.3	14
64	Exchange and correlation in the Si atom: A quantum Monte Carlo study. *Physical Review A*, **2001**, 64,	2.6	10
63	Quantum electronic stability of atomically uniform films. *Science*, **2001**, 292, 1131-3	33.3	150
62	Comment on "Determination of phonon dispersions from X-Ray transmission scattering: the example of silicon". *Physical Review Letters*, **2000**, 84, 3733	7.4	8
61	Sn/Ge(111) surface charge-density-wave phase transition. *Physical Review Letters*, **2000**, 85, 3684-7	7.4	31
60	Pair-tunneling states in semiconductor quantum dots: Ground-state behavior in a magnetic field. *Physical Review B*, **1998**, 57, 12281-12284	3.3	10
59	Exchange and correlation in silicon. *Physical Review B*, **1998**, 57, 8972-8982	3.3	89
58	Role of hydrogen in SiH2 adsorption on Si(100). *Physical Review B*, **1998**, 58, R13363-R13366	3.3	19

57	Effect of hydrogen on the surface-energy anisotropy of diamond and silicon. *Physical Review B*, **1998**, 57, 6262-6265	3.3	49
56	Elimination of Coulomb finite-size effects in quantum many-body simulations. *Physical Review B*, **1997**, 55, R4851-R4854	3.3	87
55	Quantum Monte Carlo Investigation of Exchange and Correlation in Silicon. *Physical Review Letters*, **1997**, 78, 3350-3353	7.4	61
54	Theoretical study of hydrogen-covered diamond (100) surfaces: A chemical-potential analysis. *Physical Review B*, **1997**, 55, 9975-9982	3.3	38
53	Wavelets in self-consistent electronic structure calculations. *Physical Review Letters*, **1996**, 76, 2650-2653	7.4	106
52	First-principles study of the H-induced reconstruction of W(110). *Physical Review B*, **1996**, 53, 13734-13739	3.3	22
51	Total-energy study of hydrogen ordering in PdHx (0 . *Physical Review B*, **1996**, 53, 1-4	3.3	78
50	Shell Structure in Metal Clusters. *Kluwer International Series in Engineering and Computer Science*, **1996**, 287-297		
49	Structural and electronic properties of hexagonal yttrium trihydride. *Physical Review B*, **1995**, 51, 7500-7507	3.3	52
48	Energetics and lattice contraction of beta -phase YH2+x. *Physical Review B*, **1994**, 49, 10731-10734	3.3	23
47	Pseudopotential plane-wave study of alpha -YHx. *Physical Review B*, **1994**, 49, 13357-13365	3.3	20
46	First-principles determination of equilibrium crystal shapes for metals at T=0. *Physical Review B*, **1994**, 50, 4859-4862	3.3	31
45	Tight-binding model with intra-atomic matrix elements. *Physical Review B*, **1994**, 49, 8506-8509	3.3	64
44	First-principles study of hydrogen ordering in beta -YH2+x. *Physical Review B*, **1994**, 49, 6481-6489	3.3	25
43	Continuous feedback approach for controlling chaos. *Physical Review E*, **1994**, 50, 2331-2334	2.4	23
42	Phonon dispersions of silicon and germanium from first-principles calculations. *Physical Review B*, **1994**, 50, 2221-2226	3.3	81
41	Ab initio calculation of thermodynamic properties of silicon. *Physical Review B*, **1994**, 50, 14587-14590	3.3	52
40	Asymmetric phase diagram and coverage dependent effective pair interactions for hydrogen on close-packed metal surfaces. *Surface Science*, **1993**, 280, 415-429	1.8	3

39	Peierls distortion in hexagonal YH3. *Physical Review Letters*, **1993**, 71, 1226-1229	7.4	59
38	Tight-binding total-energy models for silicon and germanium. *Physical Review B*, **1993**, 47, 9366-9376	3.3	56
37	Energetics of the Si(111) and Ge(111) surfaces and the effect of strain. *Physical Review B*, **1993**, 48, 5374-5385	3.3	20
36	Comment on "Should all surfaces be reconstructed?". *Physical Review Letters*, **1993**, 71, 461	7.4	13
35	Theoretical Study of the Binding Properties and Electronic Structure of Hydrogen in Yttrium*. *Zeitschrift Fur Physikalische Chemie*, **1993**, 181, 39-42	3.1	
34	Reformulation of generalized separable pseudopotentials. *Physical Review B*, **1992**, 45, 11465-11468	3.3	6
33	First-Principles Calculation of Force Constants and Full Phonon Dispersions. *Materials Research Society Symposia Proceedings*, **1992**, 291, 641		
32	Ab initio calculation of force constants and full phonon dispersions. *Physical Review Letters*, **1992**, 69, 2799-2802	7.4	183
31	Pseudopotential plane-wave calculation of the structural properties of yttrium. *Physical Review B*, **1991**, 44, 10339-10342	3.3	9
30	Tight-binding study of the electronic structure of amorphous silicon. *Physical Review B*, **1991**, 43, 6768-6771	3.3	19
29	A new ab initio potential energy surface for hydrogen atom on ruthenium(0001) and its use for variational transition state theory and semiclassical tunneling calculations of the surface diffusion of hydrogen and deuterium. *The Journal of Physical Chemistry*, **1990**, 94, 1973-1981		14
28	Theoretical study of hydrogen adsorption on Ru(0001): Possible surface and subsurface occupation sites. *Physical Review B*, **1989**, 39, 5623-5631	3.3	44
27	Lumping coupled nonlinear reactions in continuous mixtures. *AICHE Journal*, **1989**, 35, 533-538	3.6	34
26	Continuum theory for lumping nonlinear reactions. *AICHE Journal*, **1988**, 34, 1519-1527	3.6	59
25	Band tails, path integrals, instantons, polarons, and all that. *IBM Journal of Research and Development*, **1988**, 32, 82-92	2.5	32
24	Density of states for an electron in a correlated Gaussian random potential: Theory of the Urbach tail. *Physical Review B*, **1988**, 37, 6963-6976	3.3	49
23	Ab initio pseudopotential-local-density description of the structural properties of small carbon clusters. *Physical Review B*, **1988**, 37, 6504-6507	3.3	9
22	Electronic and structural properties of elemental copper: A pseudopotential-local-orbital calculation. *Physical Review B*, **1988**, 38, 7966-7971	3.3	41

21	First-principles study of hydrogen adsorption on Ru(0001): Possible occupation of subsurface sites. *Physical Review Letters*, **1987**, 59, 1737-1740	7.4	62
20	Structural properties of the Ru(0001) surface. *Physical Review B*, **1987**, 35, 2124-2127	3.3	19
19	Electronic shell structure of simple metal heteroclusters. *Physical Review B*, **1987**, 36, 3455-3458	3.3	52
18	Physics of metal clusters. *The Journal of Physical Chemistry*, **1987**, 91, 3141-3149		130
17	Pseudopotential approaches to the structural energies of crystalline solids and solid surfaces. *Physics and Chemistry of Minerals*, **1987**, 14, 308-314	1.6	3
16	Alkali metal clusters and the jellium model. *Chemical Physics Letters*, **1987**, 134, 1-5	2.5	69
15	Electronic shell structure in simple metal clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1986**, 113, 420-424	2.3	140
14	Ab initio study of the structural properties of magnesium. *Solid State Communications*, **1986**, 57, 785-788	1.6	25
13	Theoretical Compton profiles of graphite and LiC6. *Physical Review B*, **1986**, 33, 6619-6626	3.3	27
12	Elastic jellium sphere in a static electric field. *Physical Review B*, **1986**, 34, 732-739	3.3	10
11	Theoretical study of stacking faults in silicon. *Physical Review B*, **1985**, 32, 7979-7987	3.3	107
10	Ground-state properties of Be2: A pseudopotential local-density approach. *Physical Review A*, **1985**, 31, 3444-3446	2.6	2
9	Angle-resolved photoemission study of the electronic structure of beryllium: Bulk band dispersions and many-electron effects. *Physical Review B*, **1984**, 30, 5500-5507	3.3	47
8	Total energies, abundances, and electronic shell structure of lithium, sodium, and potassium clusters. *Solid State Communications*, **1984**, 52, 645-648	1.6	160
7	Electronic Shell Structure and Abundances of Sodium Clusters. *Physical Review Letters*, **1984**, 52, 2141-2143	7.4	2030
6	Electron momentum distribution in graphite and lithium-intercalated graphite. *Physical Review B*, **1984**, 30, 1062-1064	3.3	19
5	Temperature- and pressure-induced crystal phase transitions in Be. *Journal of Physics C: Solid State Physics*, **1984**, 17, 2065-2073		27
4	Calculation of the Compton profile of beryllium. *Physical Review B*, **1983**, 28, 1696-1700	3.3	16

3	Ab initiostudy of structural and electronic properties of beryllium. *Physical Review B*, **1983**, 28, 4179-4185	3.3	117
2	Compton Profile of Beryllium. *Physical Review Letters*, **1982**, 49, 1452-1455	7.4	36
1	Ab initio calculation of the static structural properties of Be. *Solid State Communications*, **1982**, 42, 861-863	1.8	34