Mei-Yin Chou

List of Publications by Citations

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	Electronic Shell Structure and Abundances of Sodium Clusters. *Physical Review Letters*, **1984**, 52, 2141-2143	7.4	2030
163	Janus monolayers of transition metal dichalcogenides. *Nature Nanotechnology*, **2017**, 12, 744-749	28.7	828
162	Ultrahigh-gain photodetectors based on atomically thin graphene-MoS2 heterostructures. *Scientific Reports*, **2014**, 4, 3826	4.9	678
161	Quantum confinement and electronic properties of silicon nanowires. *Physical Review Letters*, **2004**, 92, 236805	7.4	438
160	Determination of band alignment in the single-layer MoS2/WSe2 heterojunction. *Nature Communications*, **2015**, 6, 7666	17.4	421
159	Structural and electronic properties of oxidized graphene. *Physical Review Letters*, **2009**, 103, 086802	7.4	408
158	Interlayer couplings, Moir patterns, and 2D electronic superlattices in MoS/WSe hetero-bilayers. *Science Advances*, **2017**, 3, e1601459	14.3	277
157	Oxidation functional groups on graphene: Structural and electronic properties. *Physical Review B*, **2010**, 82,	3.3	272
156	Theory of quantum size effects in thin Pb(111) films. *Physical Review B*, **2002**, 66,	3.3	244
155	Persistent superconductivity in ultrathin Pb films: a scanning tunneling spectroscopy study. *Physical Review Letters*, **2006**, 96, 027005	7.4	232
154	Ca3P2 and other topological semimetals with line nodes and drumhead surface states. *Physical Review B*, **2016**, 93,	3.3	230
153	Ultrahigh thermoelectric performance in Cu2Se-based hybrid materials with highly dispersed molecular CNTs. *Energy and Environmental Science*, **2017**, 10, 1928-1935	35.4	215
152	Ab initio calculation of force constants and full phonon dispersions. *Physical Review Letters*, **1992**, 69, 2799-2802	7.4	183
151	Alternative low-symmetry structure for 13-atom metal clusters. *Physical Review Letters*, **2004**, 93, 133401	7.4	181
150	Phonon dispersions and vibrational properties of monolayer, bilayer, and trilayer graphene: Density-functional perturbation theory. *Physical Review B*, **2008**, 77,	3.3	170
149	Electron-hole coupling and the charge density wave transition in TiSe2. *Physical Review Letters*, **2002**, 88, 226402	7.4	161
148	Total energies, abundances, and electronic shell structure of lithium, sodium, and potassium clusters. *Solid State Communications*, **1984**, 52, 645-648	1.6	160

147	Charge density wave transition in single-layer titanium diselenide. *Nature Communications*, **2015**, 6, 8943	17.4	154
146	Stability and electronic properties of two-dimensional silicene and germanene on graphene. *Physical Review B*, **2013**, 88,	3.3	153
145	Quantum electronic stability of atomically uniform films. *Science*, **2001**, 292, 1131-3	33.3	150
144	Thermal stability and electronic structure of atomically uniform Pb films on Si(111). *Physical Review Letters*, **2004**, 93, 026802	7.4	143
143	Electronic shell structure in simple metal clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1986**, 113, 420-424	2.3	140
142	Effects of metallic contacts on electron transport through graphene. *Physical Review Letters*, **2010**, 104, 076807	7.4	130
141	Physics of metal clusters. *The Journal of Physical Chemistry*, **1987**, 91, 3141-3149		130
140	Ab initiostudy of structural and electronic properties of beryllium. *Physical Review B*, **1983**, 28, 4179-4185	3.3	117
139	X-ray studies of phonon softening in tise2. *Physical Review Letters*, **2001**, 86, 3799-802	7.4	110
138	Theoretical study of stacking faults in silicon. *Physical Review B*, **1985**, 32, 7979-7987	3.3	107
137	Wavelets in self-consistent electronic structure calculations. *Physical Review Letters*, **1996**, 76, 2650-2653	7.4	106
136	Size and orientation dependence in the electronic properties of silicon nanowires. *Physical Review B* , **2007**, 76,	3.3	93
135	Electron-phonon coupling in two-dimensional silicene and germanene. *Physical Review B*, **2013**, 88,	3.3	92
134	Unique Gap Structure and Symmetry of the Charge Density Wave in Single-Layer VSe_{2}. *Physical Review Letters*, **2018**, 121, 196402	7.4	90
133	Exchange and correlation in silicon. *Physical Review B*, **1998**, 57, 8972-8982	3.3	89
132	Elimination of Coulomb finite-size effects in quantum many-body simulations. *Physical Review B*, **1997**, 55, R4851-R4854	3.3	87
131	Spin texture in type-II Weyl semimetal WTe2. *Physical Review B*, **2016**, 94,	3.3	83
130	Atomic-layer-resolved quantum oscillations in the work function: Theory and experiment for Ag/Fe(100). *Physical Review B*, **2002**, 66,	3.3	82

129	Phonon dispersions of silicon and germanium from first-principles calculations. *Physical Review B*, **1994**, 50, 2221-2226	3.3	81
128	First-principles study of NaAlH4 and Na3AlH6 complex hydrides. *Physical Review B*, **2004**, 70,	3.3	78
127	Alternating layer and island growth of Pb on Si by spontaneous quantum phase separation. *Physical Review Letters*, **2003**, 90, 076104	7.4	78
126	Total-energy study of hydrogen ordering in PdHx (0 . *Physical Review B*, **1996**, 53, 1-4	3.3	78
125	Large quantum-spin-Hall gap in single-layer 1TNWSe. *Nature Communications*, **2018**, 9, 2003	17.4	74
124	Elemental Topological Dirac Semimetal: Sn on InSb(111). *Physical Review Letters*, **2017**, 118, 146402	7.4	71
123	Fractal Landau-level spectra in twisted bilayer graphene. *Nano Letters*, **2012**, 12, 3833-8	11.5	70
122	Alkali metal clusters and the jellium model. *Chemical Physics Letters*, **1987**, 134, 1-5	2.5	69
121	Gapped electronic structure of epitaxial stanene on InSb(111). *Physical Review B*, **2018**, 97,	3.3	68
120	Quantum confinement effect in Si/Ge core-shell nanowires: First-principles calculations. *Physical Review B*, **2008**, 77,	3.3	64
119	Tight-binding model with intra-atomic matrix elements. *Physical Review B*, **1994**, 49, 8506-8509	3.3	64
118	Emergence of charge density waves and a pseudogap in single-layer TiTe. *Nature Communications*, **2017**, 8, 516	17.4	63
117	First-principles study of hydrogen adsorption on Ru(0001): Possible occupation of subsurface sites. *Physical Review Letters*, **1987**, 59, 1737-1740	7.4	62
116	Quantum Monte Carlo Investigation of Exchange and Correlation in Silicon. *Physical Review Letters*, **1997**, 78, 3350-3353	7.4	61
115	Peierls distortion in hexagonal YH3. *Physical Review Letters*, **1993**, 71, 1226-1229	7.4	59
114	Continuum theory for lumping nonlinear reactions. *AICHE Journal*, **1988**, 34, 1519-1527	3.6	59
113	Enhanced electron-hole interaction and optical absorption in a silicon nanowire. *Physical Review B*, **2007**, 75,	3.3	57
112	Tight-binding total-energy models for silicon and germanium. *Physical Review B*, **1993**, 47, 9366-9376	3.3	56

111	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
110	Structural and electronic properties of hexagonal yttrium trihydride. *Physical Review B*, **1995**, 51, 7500-7507	3.3	52
109	Ab initio calculation of thermodynamic properties of silicon. *Physical Review B*, **1994**, 50, 14587-14590	3.3	52
108	Electronic shell structure of simple metal heteroclusters. *Physical Review B*, **1987**, 36, 3455-3458	3.3	52
107	Bandgap renormalization and work function tuning in MoSe/hBN/Ru(0001) heterostructures. *Nature Communications*, **2016**, 7, 13843	17.4	51
106	Stable 1T Tungsten Disulfide Monolayer and Its Junctions: Growth and Atomic Structures. *ACS Nano*, **2018**, 12, 12080-12088	16.7	51
105	Effect of hydrogen on the surface-energy anisotropy of diamond and silicon. *Physical Review B*, **1998**, 57, 6262-6265	3.3	49
104	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
103	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
102	Dimensional Effects on the Charge Density Waves in Ultrathin Films of TiSe. *Nano Letters*, **2016**, 16, 6331-6336	11.5	46
101	Theoretical study of hydrogen adsorption on Ru(0001): Possible surface and subsurface occupation sites. *Physical Review B*, **1989**, 39, 5623-5631	3.3	44
100	Electronic and structural properties of elemental copper: A pseudopotential-local-orbital calculation. *Physical Review B*, **1988**, 38, 7966-7971	3.3	41
99	Electron-phonon interactions for optical-phonon modes in few-layer graphene: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	38
98	Theoretical study of hydrogen-covered diamond (100) surfaces: A chemical-potential analysis. *Physical Review B*, **1997**, 55, 9975-9982	3.3	38
97	Strong Asymmetric Charge Carrier Dependence in Inelastic Electron Tunneling Spectroscopy of Graphene Phonons. *Physical Review Letters*, **2015**, 114, 245502	7.4	37
96	Phase relations associated with one-dimensional shell effects in thin metal films. *Physical Review Letters*, **2009**, 102, 236803	7.4	37
95	Fermi surfaces and energy gaps in Sn/Ge(111). *Journal of Physics Condensed Matter*, **2002**, 14, R1-R20	1.8	37
94	Compton Profile of Beryllium. *Physical Review Letters*, **1982**, 49, 1452-1455	7.4	36

93	Effects of the substrate on quantum well states: A first-principles study for Ag/Fe(100). *Physical Review B*, **2003**, 68,	3.3	34
92	Hydrogenation-induced insulating state in the intermetallic compound LaMg2Ni. *Physical Review Letters*, **2005**, 94, 066403	7.4	34
91	Lumping coupled nonlinear reactions in continuous mixtures. *AICHE Journal*, **1989**, 35, 533-538	3.6	34
90	Ab initio calculation of the static structural properties of Be. *Solid State Communications*, **1982**, 42, 861-863	1.6	34
89	Effects of electrostatic fields and charge doping on the linear bands in twisted graphene bilayers. *Physical Review B*, **2011**, 84,	3.3	32
88	Band tails, path integrals, instantons, polarons, and all that. *IBM Journal of Research and Development*, **1988**, 32, 82-92	2.5	32
87	Strain Engineering a 4□ Charge Density Wave Phase in Transition Metal Dichalcogenide 1T-VSe. *Physical Review Materials*, **2017**, 1,	3.2	32
86	Sn/Ge(111) surface charge-density-wave phase transition. *Physical Review Letters*, **2000**, 85, 3684-7	7.4	31
85	First-principles determination of equilibrium crystal shapes for metals at T=0. *Physical Review B*, **1994**, 50, 4859-4862	3.3	31
84	End-Bonded Metal Contacts on WSe Field-Effect Transistors. *ACS Nano*, **2019**, 13, 8146-8154	16.7	30
83	Thermoelectric Figure-of-Merit of Fully Dense Single-Crystalline SnSe. *ACS Omega*, **2019**, 4, 5442-5450	3.9	28
82	First-principles studies of quasiparticle band structures of cubic YH3 and LaH3. *Physical Review B*, **2003**, 67,	3.3	28
81	Theoretical Compton profiles of graphite and LiC6. *Physical Review B*, **1986**, 33, 6619-6626	3.3	27
80	Temperature- and pressure-induced crystal phase transitions in Be. *Journal of Physics C: Solid State Physics*, **1984**, 17, 2065-2073		27
79	Ultrafast Monolayer In/Gr-WS-Gr Hybrid Photodetectors with High Gain. *ACS Nano*, **2019**, 13, 3269-3279	16.7	26
78	First-principles study of hydrogen ordering in beta -YH2+x. *Physical Review B*, **1994**, 49, 6481-6489	3.3	25
77	Ab initio study of the structural properties of magnesium. *Solid State Communications*, **1986**, 57, 785-788	1.6	25
76	Hidden Order and Dimensional Crossover of the Charge Density Waves in TiSe. *Scientific Reports*, **2016**, 6, 37910	4.9	24

75	Size- and Strain-Dependent Electronic Structures in H-Passivated Si [112] Nanowires. *Journal of Physical Chemistry C*, **2008**, 112, 15680-15683	3.8	24
74	Electronic and vibrational properties of AlH3. *Physical Review B*, **2008**, 77,	3.3	23
73	Energetics and lattice contraction of beta -phase YH2+x. *Physical Review B*, **1994**, 49, 10731-10734	3.3	23
72	Continuous feedback approach for controlling chaos. *Physical Review E*, **1994**, 50, 2331-2334	2.4	23
71	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
70	First-principles study of the H-induced reconstruction of W(110). *Physical Review B*, **1996**, 53, 13734-13739	3.3	22
69	Quantum size effect in Pb(100) films: Critical role of crystal band structure. *Physical Review B*, **2007**, 75,	3.3	21
68	Energetics of the Si(111) and Ge(111) surfaces and the effect of strain. *Physical Review B*, **1993**, 48, 5374-5385	3.3	20
67	Pseudopotential plane-wave study of alpha -YHx. *Physical Review B*, **1994**, 49, 13357-13365	3.3	20
66	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
65	Role of hydrogen in SiH2 adsorption on Si(100). *Physical Review B*, **1998**, 58, R13363-R13366	3.3	19
64	Tight-binding study of the electronic structure of amorphous silicon. *Physical Review B*, **1991**, 43, 6768-6771	3.3	19
63	Structural properties of the Ru(0001) surface. *Physical Review B*, **1987**, 35, 2124-2127	3.3	19
62	Electron momentum distribution in graphite and lithium-intercalated graphite. *Physical Review B*, **1984**, 30, 1062-1064	3.3	19
61	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
60	In Situ Strain Tuning of the Dirac Surface States in BiSe Films. *Nano Letters*, **2018**, 18, 5628-5632	11.5	17
59	Tailoring Semiconductor Lateral Multijunctions for Giant Photoconductivity Enhancement. *Advanced Materials*, **2017**, 29, 1703680	24	17
58	Lattice vibrational modes and their frequency shifts in semiconductor nanowires. *Nano Letters*, **2011**, 11, 2618-21	11.5	17

57	Catalytic effect of near-surface alloying on hydrogen interaction on the aluminum surface. *Physical Review B*, **2011**, 83,	3.3	17
56	Lattice dynamics and thermodynamic properties of NaAlH4: Density-functional calculations using a linear response theory. *Physical Review B*, **2006**, 73,	3.3	17
55	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
54	Charge transport through graphene junctions with wetting metal leads. *Nano Letters*, **2012**, 12, 3424-30	11.5	16
53	Enhanced optical conductivity induced by surface states in ABC-stacked few-layer graphene. *Physical Review B*, **2011**, 83,	3.3	16
52	Diffusion of Si and C atoms on and between graphene layers. *Journal Physics D: Applied Physics*, **2012**, 45, 455309	3	16
51	Calculation of the Compton profile of beryllium. *Physical Review B*, **1983**, 28, 1696-1700	3.3	16
50	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. *Physical Review B*, **2012**, 85,	3.3	15
49	Coupled Dirac fermions and neutrino-like oscillations in twisted bilayer graphene. *Nano Letters*, **2013**, 13, 5159-64	11.5	14
48	Comparative study of density-functional theories of the exchange-correlation hole and energy in silicon. *Physical Review B*, **2001**, 64,	3.3	14
47	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
46	Surface passivation and orientation dependence in the electronic properties of silicon nanowires. *Journal of Physics Condensed Matter*, **2013**, 25, 145501	1.8	13
45	Path to Wigner localization in circular quantum dots. *Physical Review B*, **2009**, 79,	3.3	13
44	Comment on "Should all surfaces be reconstructed?". *Physical Review Letters*, **1993**, 71, 461	7.4	13
43	Epitaxial Growth of Two-Dimensional Insulator Monolayer Honeycomb BeO. *ACS Nano*, **2021**, 15, 2497-2505	13.7	13
42	Low-lying spectra of massless Dirac electron in magnetic dot and ring. *Applied Physics Letters*, **2010**, 96, 212101	3.4	12
41	Topological Properties of Gapped Graphene Nanoribbons with Spatial Symmetries. *Nano Letters*, **2018**, 18, 7254-7260	11.5	12
40	LaMg2PdH7, a new complex metal hydride containing tetrahedral [PdH4]4□anions. *Journal of Alloys and Compounds*, **2007**, 446-447, 34-38	5.7	11

39	Anomalous phase relations of quantum size effects in ultrathin Pb films on Si(111). *Physical Review B*, **2013**, 87,	3.3	10
38	Exchange and correlation in the Si atom: A quantum Monte Carlo study. *Physical Review A*, **2001**, 64,	2.6	10
37	Pair-tunneling states in semiconductor quantum dots: Ground-state behavior in a magnetic field. *Physical Review B*, **1998**, 57, 12281-12284	3.3	10
36	Elastic jellium sphere in a static electric field. *Physical Review B*, **1986**, 34, 732-739	3.3	10
35	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
34	First-principles investigation of sodium and lithium alloyed alanates. *Journal of Alloys and Compounds*, **2009**, 479, 678-683	5.7	9
33	Low-energy ordered structures of Li2Mg(NH)2. *Journal of Applied Physics*, **2008**, 104, 083519	2.5	9
32	Pseudopotential plane-wave calculation of the structural properties of yttrium. *Physical Review B*, **1991**, 44, 10339-10342	3.3	9
31	Ab initio pseudopotential-local-density description of the structural properties of small carbon clusters. *Physical Review B*, **1988**, 37, 6504-6507	3.3	9
30	Electrical valley filtering in transition metal dichalcogenides. *Physical Review Materials*, **2018**, 2,	3.2	9
29	Theory of valley-dependent transport in graphene-based lateral quantum structures. *Physical Review B*, **2016**, 94,	3.3	9
28	Comment on "Determination of phonon dispersions from X-Ray transmission scattering: the example of silicon". *Physical Review Letters*, **2000**, 84, 3733	7.4	8
27	Liquidlike Cu atom diffusion in weakly ionic compounds Cu2S and Cu2Se. *Physical Review B*, **2020**, 102,	3.3	8
26	Quantum Monte Carlo investigations of adsorption energetics on graphene. *Journal of Physics Condensed Matter*, **2012**, 24, 395002	1.8	7
25	Zhao et al. Reply:. *Physical Review Letters*, **2005**, 94,	7.4	7
24	Kidd et al. Reply:. *Physical Review Letters*, **2002**, 88,	7.4	7
23	Exchange-correlation energy in molecules: A variational quantum Monte Carlo study. *Physical Review A*, **2006**, 74,	2.6	6
22	Reformulation of generalized separable pseudopotentials. *Physical Review B*, **1992**, 45, 11465-11468	3.3	6

21	Theoretical study of quantum size effects in thin Al(100), Al(110), and Al(111) films. *Physical Review B*, **2019**, 99,	3.3	5
20	Theoretical investigation of intermediate phases between Li2NH and LiNH2. *Physical Review B*, **2010**, 82,	3.3	5
19	Ultrafast Bulk Diffusion of AlHx in High-Entropy Dehydrogenation Intermediates of NaAlH4. *Journal of Physical Chemistry C*, **2014**, 118, 18356-18361	3.8	3
18	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
17	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
16	Optical phonon anomaly in Bernal stacked bilayer graphene with ultrahigh carrier densities. *Physical Review B*, **2012**, 86,	3.3	3
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14	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
13	Pseudopotential approaches to the structural energies of crystalline solids and solid surfaces. *Physics and Chemistry of Minerals*, **1987**, 14, 308-314	1.6	3
12	Theoretical study of the vibrational properties of NaAlH4 with AlH3 vacancies. *Faraday Discussions*, **2011**, 151, 243-51; discussion 285-95	3.6	2
11	Stability of the hydrogen-storage compound Li6Mg(NH)4 from first principles. *Physical Review B*, **2011**, 83,	3.3	2
10	Ground-state properties of Be2: A pseudopotential local-density approach. *Physical Review A*, **1985**, 31, 3444-3446	2.6	2
9	Origin of Band Modulation in GeTe-Rich Ge□Sb□Te Thin Film. *ACS Applied Electronic Materials*, **2019**, 1, 2619-2625	4	2
8	Coherent Electronic Band Structure of TiTe/TiSe Moiré Bilayer. *ACS Nano*, **2021**, 15, 3359-3364	16.7	1
7	Mechanism for anisotropic diffusion of liquid-like Cu atoms in hexagonal □u2S. *Physical Review Materials*, **2021**, 5,	3.2	1
6	Structure Relaxation and Liquidlike Enhanced Cu Diffusion at the Surface of □CuS Chalcocite. *Nano Letters*, **2021**, 21, 8895-8900	11.5	0
5	Embedment of Multiple Transition Metal Impurities into WS Monolayer for Bandstructure Modulation. *Small*, **2021**, 17, e2007171	11	0
4	Theoretical Study of the Binding Properties and Electronic Structure of Hydrogen in Yttrium*. *Zeitschrift Fur Physikalische Chemie*, **1993**, 181, 39-42	3.1	

List of Publications

3	First-Principles Calculation of Force Constants and Full Phonon Dispersions. *Materials Research Society Symposia Proceedings*, **1992**, 291, 641	
2	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
1	Shell Structure in Metal Clusters. *Kluwer International Series in Engineering and Computer Science*, **1996**, 287-297	