

Masoud Javan, PhD

Associate Professor of Physics & Solid State Physics
Faculty of Science, Department of Physics
Golestan University

Academic Profile

Distinguished computational physicist with extensive expertise in density functional theory (DFT), molecular dynamics, and nanomaterial simulation. Research focuses on quantum mechanical analysis of nanomaterials for drug delivery, sensor applications, and renewable energy. Extensive publication record with over 60 peer-reviewed articles in high-impact journals. Committed to advancing theoretical nanoscience through interdisciplinary collaboration and innovative computational methodologies.

Complete Publication Record *(2008-2025)*

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2008	تجبر، مهدی؛ بزی جوان سرگزایی	ویژگی های مغناطیسی نانوسیم (Cr, Mn, Fe, Co, Ni) های فلزات واسط	شانزدهمین همایش بلورشناسی و کانی شناسی ایران	-	-	-
2010	Javan, M Bezi; Tajabor, Nasser; Behdani, Mohammad; Rokn-Abadi, M Rezaee	Influence of 3d transition metals (Fe, Co) on the structural, electrical and magnetic properties of C60 nano-cage	Physica B: Condensed Matter	405/24	4937- 4942	45
2011	Javan, M Bezi; Tajabor, Nasser; Rezaee-Roknabadi, Mahmood; Behdani, Mohammad	First principles study of small cobalt clusters encapsulated in C60 and C82 spherical nanocages	Applied Surface Science	257/17	7586- 7591	67

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2011	Javan, M Bezi; Tajabor, Nasser; Roknabadi, M Rezaee; Behdani, Mohammad	First principles calculations of C70 fullerene nano-cage doped with transition metal atoms (Fe, Co)	Physica E: Low-dimensional Systems and Nanostructures	43/7	1351-1359	52
2011	Javan, M Bezi; Ganji, MD; Sabet, M; Danesh, N	Incorporation of hydrogen molecules into carbon nitride heterofullerenes: an Ab initio study	Journal of Computational and Theoretical Nanoscience	8/5	803-807	18
2011	تجبر، رضائی، یزى جوان رکن آبادی، بهدانی	بررسی ساختاری، الکترونی و مغناطیسی نانو خوشه های آهن و کبالت	نوزدهمین همایش بلورشناسی و کانیشناسی ایران	-	-	-
2012	Javan, M Bezi; Tajabor, Nasser	Structural, electronic and magnetic properties of Fen@ C60 and	Journal of Magnetism and Magnetic Materials	324/1	52-59	71

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		Fen@ C80 (n= 2–7) endohedral metallofullerene nano-cages: First principles study				
2012	Javan, Masoud Bezi	First principles study of the electronic and optical properties of GaAs nanoparticles under the influence of external uniform electric field	Physics Letters A	376/45	3241- 3247	28
2013	Javan, Masoud Bezi; Ganji, Masoud Darvish	Theoretical investigation on the encapsulation of atomic hydrogen into heterofullerene nanocages	Current Applied Physics	13/7	1525- 1531	22

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2013	Bezi Javan, Masoud	Oxygen doped SiC nanocrystals: first principles study of the optical properties	Journal of Molecular Modeling	19/9	3603-3610	35
2013	Javan, Masoud Bezi	Electronic and optical properties of nitrogen doped SiC nanocrystals: first principles study	International Journal of Modern Physics B	27/13	13500-53	29
2013	Bezi Javan, Masoud	Optical properties of SiC nanocages: ab initio study	Applied Physics A	113/1	105-113	42
2013	Javan, Masoud Bezi	Optical properties of GaAs nanocrystals: influence of an electric field	Journal of Molecular Modeling	19/6	2273-2283	31

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2013	Javan, Masoud Bezi	Ab initio study of the nitrogen doped Si ₄₃ C ₄₄ H ₇₆ nanoparticle: Time-dependent density functional theory	Thin Solid Films	534	535-540	24
2014	Bezi Javan, Masoud; Ebrahimi, Samaneh	Structural, electronic and magnetic properties of C ₅₉ Ir, C ₅₈ Ir ₂ , and C ₆₉ Ir heterofullerene nano-cages: first principles study	Applied Physics A	114/2	529-536	19
2014	Javan, Masoud Bezi	Small cobalt clusters encapsulated inside Si ₃₀ C ₃₀ nanocages: electronic and magnetic properties	Journal of Molecular Modeling	20/3	2145	27

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2014	Javan, Masoud Bezi	Fullerene-like Si60C60 nanocage: Hydrogen storage capacity	Current Applied Physics	14/3	484-490	33
2014	Javan, Mehran Honarmand; Haghshenas, Sina Shaffiee; Javan, Masoud Honarmand; Jalilvand, Pooria	Investigation of the Effect of Mass Super Structure in Reaction Single Micropile under Dynamic Loading	Advances in Soil Dynamics and Foundation Engineering	-	425-432	8
2015	Javan, Masoud Bezi	Surface passivation effects on the electronic and optical properties of 3C-SiC nanocrystals	Physica B: Condensed Matter	456	321-329	26
2015	Javan, Masoud Bezi	Electronic transport properties of linear nC20 ($n \leq 5$) oligomers:	Physica E: Low-Dimensional Systems and	67	135-142	21

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		Theoretical investigation	Nanostructures			
2015	Javan, Masoud Bezi	Adsorption of CO and NO molecules on SiC nanotubes and nanocages: DFT study	Surface Science	635	128-142	48
2015	Javan, Masoud Bezi	Magnetic properties of Mg ₁₂ O ₁₂ nanocage doped with transition metal atoms (Mn, Fe, Co and Ni): DFT study	Journal of Magnetism and Magnetic Materials	385	138-144	37
2015	Javan, Masoud Bezi; Orimi, Rahim Lotfi	Electric field and phosphorus doping roles on the electronic and optical properties of	Journal of Computational and Theoretical Nanoscience	12/6	1023-1029	15

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		SiC Nanocrystals: First principles study				
2015	Javan, Masoud Bezi	Structural, electronic and magnetic properties of small bimetallic zirconium– palladium clusters: ab initio study	Journal of Alloys and Compounds	643	56-63	24
2015	Javan, Masoud Bezi	Ge–Si and Si–Ge core–shell nanocrystals: Theoretical study	Thin Solid Films	589	120- 124	19
2015	Soltani, Alireza; Javan, Masoud Bezi	Carbon monoxide interactions with pure and doped B11XN12 (X= Mg, Ge, Ga) nano-	RSC Advances	5/110	90621 - 90631	41

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		clusters: a theoretical study				
2016	Javan, Masoud Bezi	Electronic and magnetic properties of monolayer SiC sheet doped with 3d-transition metals	Journal of Magnetism and Magnetic Materials	401	656-661	33
2016	Soltani, Alireza; Azmoodeh, Zivar; Javan, Masoud Bezi; Lemeski, E Tazikeh; Karami, Leila	A DFT study of adsorption of glycine onto the surface of BC2N nanotube	Applied Surface Science	384	230-236	46
2016	Soltani, Alireza; Sousaraei, Ahmad; Javan, Masoud Bezi; Eskandari, Mortaza; Balakheyli, Hanzaleh	Electronic and optical properties of 5-AVA-functionalized BN nanoclusters: a DFT study	New Journal of Chemistry	40/8	7018-7026	52

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2016	Javan, Masoud Bezi; Soltani, Alireza; Lemeski, E Tazikeh; Ahmadi, Afsaneh; Rad, Sahar Moazen	Interaction of B12N12 nano-cage with cysteine through various functionalities: a DFT study	Superlattices and Microstructure s	100	24-37	64
2016	Javan, Masoud Bezi; Shirdel-Havar, Amir Houshang; Soltani, Alireza; Pourarian, Faiz	Adsorption and dissociation of H2 on Pd doped graphene-like SiC sheet	International Journal of Hydrogen Energy	41/48	22886 - 22898	38
2016	Javan, Masoud Bezi; Soltani, Alireza; Azmoodeh, Zivar; Abdolahi, Nafiseh; Gholami, Niloofar	A DFT study on the interaction between 5-fluorouracil and B12N12 nanocluster	RSC Advances	6/106	10451 3- 10452 1	150+
2016	Javan, Masoud Bezi; Soltani, Alireza; Azmoodeh, Zivar;	A DFT study on the interaction between	-	-	-	-

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Abdolahi, Nafiseh; Gholami, Niloofar	5-fluorouracil and B ₁₂ N ₁₂ nanocluster				
2017	Katin, Konstantin P; Javan, Masoud Bezi ; Maslov, Mikhail M; Soltani, Alireza	Effect of the embedded atom on the electronic, optical properties and kinetic stability of [3, 6] silaprismane	Chemical Physics	487	59-66	23
2017	Javan, Masoud Bezi ; Soltani, Alireza; Ghasemi, AS; Lemeski, E Tazikeh; Gholami, Niloofar; Balakheyli, Hanzaleh	Ga-doped and antisite double defects enhance the sensitivity of boron nitride nanotubes towards Soman and Chlorosoman	Applied Surface Science	411	1-10	29
2017	Soltani, Alireza; Javan, M Bezi ; Hoseininezhad-	Interaction of hydrogen with Pd- and co-decorated	Synthetic Metals	234	1-8	18

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Namin, Mir Saleh; Tajabor, N; Lemeski, E Tazikeh; Pourarian, Faiz	C24 fullerenes: density functional theory study				
2018	Soltani, Alireza; Taghartapeh, Mohammad Ramezani; Javan, Masoud Bezi; Mahon, Peter J; Azmoodeh, Zivar; Lemeski, E Tazikeh; Kityk, IV	Theoretical studies of hydrazine detection by pure and Al defected MgO nanotubes	Physica E: Low- dimensional Systems and Nanostructure s	97	239- 249	36
2018	Soltani, Alireza; Javan, Masoud Bezi; Baei, Mohammad T; Azmoodeh, Zivar	Adsorption of chemical warfare agents over C24 fullerene: effects of decoration of cobalt	Journal of Alloys and Compounds	735	2148- 2161	42

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2018	Soltani, Alireza; Javan, Masoud Bezi; Raz, Shima Ghafouri; Mashkoor, Reza; Khalaji, Aliakbar Dehno; Dusek, Michal; Fejfarova, Karla; Palatinus, Lukas; Rohlicek, Jan; Machek, Pavel	Crystallography, vibrational, electronic and optical analysis of 4-Bromo-2-(2, 5-dichloro-phenylimino)-phenol	Journal of Molecular Structure	1173	521-530	17
2018	Soltani, Alireza; Taghartapeh, Mohammad Ramezani; Erfani-Moghadam, Vahid; Javan, Masoud Bezi; Heidari, Fatemeh; Aghaei, Mehrdad; Mahon, Peter J	Serine adsorption through different functionalities on the B12N12 and Pt-B12N12 nanocages	Materials Science and Engineering: C	92	216-227	44

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2018	Tazikeh-Lemeski, Elham ; Soltani, Alireza; Baei, Mohammad Taghi; Javan, Masoud Bezi ; Rad, Sahar Moazen	Theoretical study on pure and doped B12N12 fullerenes as thiophene sensor	Adsorption	24/6	585-593	26
2018	Tazikeh-Lemeski, Elham ; Soltani, Alireza	Mohammad Taghi Baei, Masoud Bezi Javan & Sahar Moazen Rad	Adsorption	24	585-593	-
2019	Hassanian, Marziyeh ; Aryapour, Hassan; Goudarzi, Alireza; Javan, Masoud Bezi	Are zinc oxide nanoparticles safe? A structural study on human serum albumin using in vitro and in silico methods	Journal of Biomolecular Structure and Dynamics	39/1	330-335	31
2019	Soltani, Alireza ; Ghasemi, AS; Javan, M	Adsorption of HCOH and H ₂ S	Adsorption	25/2	235-245	28

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Bezi ; Ashrafi, F; Ince, Joshua Charles; Heidari, Fatemeh	molecules on Al ₁₂ P ₁₂ fullerene: a DFT study				
2019	Abdolhi, N ; Aghaei, M; Soltani, A; Mighani, H; Ghaemi, EA; Javan, MB ; Khalaji, AD; Sharbati, S; Shafipour, M; Balakheyli, H	Synthesis and antibacterial activities of novel Hg (II) and Zn (II) complexes of bis (thiosemicarbazone) acenaphthenequinone loaded to MWCNTs	Journal of Structural Chemistry	60/5	845-853	12
2019	Lemeski, E Tazikeh; Javan, Masoud Bezi ; Soltani, Alireza; Azmoodeh, Zivar	Optical and electronic properties of Al-doped Mg ₁₂ O ₁₂ nanocluster: a theoretical study	Russian Journal of Inorganic Chemistry	64/6	762-769	16

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2019	Katin, Konstantin P; Javan, Masoud B; Kochaev, Alexey I; Soltani, Alireza; Maslov, Mikhail M	Kinetic Stability and Reactivity of Silicon and Fluorine-Containing CL-20 Derivatives	ChemistrySelect	4/33	9659-9665	14
2019	Ostad, Fahimeh Zargari; Ghazi, ME; Javan, M; Izadifard, Morteza	DFT study of Ptn, Pdn, and Irn (n= 5, 6) clusters adsorbed on graphene: Structural and electronic properties	Physica B: Condensed Matter	575	411678	21
2020	Soltani, Alireza; Tazikeh-Lemeski, Elham; Javan, Masoud Bezi	A comparative theoretical study on the interaction of pure and carbon atom substituted boron nitride fullerenes with ifosfamide drug	Journal of Molecular Liquids	297	111894	47

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2020	Javan, Masoud; Jorjani, Roza; Soltani, Ali Reza	Theoretical study of nitrogen, boron, and co-doped (B, N) armchair graphene nanoribbons	Journal of Molecular Modeling	26/4	64	22
2020	Abdollahi, Nafiseh; Javan, Masoud Bezi; Katin, Konstantin P; Soltani, Alireza; Shojaee, Shamim; Kaveh, Sara	The study of thiazole adsorption upon BC2N nanotube: DFT/TD- DFT investigation	Structural Chemistry	31/5	1959- 1967	18
2020	Soltani, Alireza; Ramezanitaghartapeh, Mohammad; Javan, Masoud Bezi; Baei, Mohammad T; Lup, Andrew Ng Kay; Mahon, Peter J; Aghaei, Mehrdad	Influence of the adsorption of toxic agents on the optical and electronic properties of B12N12 fullerene in the presence and absence of an	New Journal of Chemistry	34/34	14513 - 14528	33

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		external electric field				
2020	Abdolahi, Nafiseh ; Singla, Preeti; Soltani, Alireza; Javan, M ; Aghaei, Mehrdad; Heidari, Fatemeh; Sedighi, Sima	Gold decorated B12N12 nanocluster as an effective sulfasalazine drug carrier: A theoretical investigation	Physica E: Low-Dimensional Systems and Nanostructures	124	11429-6	39
2020	Sedighi, Sima ; Baei, Mohammad T; Javan, Masoud ; Ince, Joshua Charles; Soltani, Alireza; Jokar, Mohammad Hassan; Tavassoli, Samaneh	Adsorption of sarin and chlorosarin onto the Al12N12 and Al12P12 nanoclusters: DFT and TDDFT calculations	Surface and Interface Analysis	52/11	725-734	24
2020	Sohraby, Farzin ; Soltanabad, Mojtaba Hadi; Bagheri, Milad; Javan, Masood	Application of molecular dynamics in coating Ag-conjugated	Nano Biomed Eng	12/1	90-98	15

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Bezi ; Moghadam, Mostafa Javaheri; Baghkheirati, Eisa Kohan; Najjar, Mohammad Bagher Bagherieh	nanoparticles with potential therapeutic applications				
2020	Zargari, Fahimeh; Javan, Masoud ; Ghazi, ME; Izadifard, Morteza	Graphene-like boron nitride supported Irn, Pdn, and Ptn (n= 5, 6) clusters: A DFT study	Diamond and Related Materials	110	108110	19
2021	Cao, Yan ; Khan, Afrasyab; Mirzaei, Hassan; Khandoozi, Seyed Reza; Javan, Masoud ; Lup, Andrew Ng Kay; Norouzi, Alireza; Lemeski, E Tazikeh; Pishnamazi,	Investigations of adsorption behavior and anti-cancer activity of curcumin on pure and platinum-functionalized B12N12 nanocages	Journal of Molecular Liquids	334	116516	58

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Maedeh; Soltani, Alireza					
2021	Majidinia, Reza; Ghazi, ME; Javan, M; Izadifard, Morteza	Effects of Zn substitution on electronic and magnetic properties of GaFeO ₃ multiferroic using density functional theory	Computational Condensed Matter	28	e0056 7	12
2021	Aghaei, Mehrdad; Ramezanitaghartapeh, Mohammad; Javan, Masoud; Hoseininezhad-Namin, Mir Saleh; Mirzaei, Hassan; Rad, Ali Shokuhi; Soltani, Alireza; Sedighi, Sima;	Investigations of adsorption behavior and anti- inflammatory activity of glycine functionalized Al ₁₂ N ₁₂ and Al ₁₂ O ₁₁ fullerene-like cages	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	246	11902 3	37

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Lup, Andrew Ng Kay; Khor, Vahid					
2021	Cao, Yan ; Khan, Afrasyab; Javan, M ; Baei, Mohammad T; Tazikeh-Lemeski, Elham; Azmoodeh, Zivar; Soltani, Alireza; Heidari, Fatemeh; Pishnamazi, Marieh; Albadarin, Ahmad B	Adsorption behavior of uracil on external surface of MgO nanotubes: A new class of hybrid nano-bio materials	Journal of Molecular Liquids	339	11673 2	28
2021	Cao, Yan ; Khan, Afrasyab; Tazikeh-Lemeski, Elham; Javan, Masoud ; Baei, Mohammad T; Taghartapeh, Mohammad Ramezani; Mighani, Hossein; Soltani, Alireza;	Modeling and simulation of external electric field application for diisopropyl methylphosphonate sensing through B12N12 fullerene	Journal of Molecular Liquids	340	11684 5	25

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
	Pishnamazi, Maedeh; Nouri, Amirhossein					
2021	Gao, Shujuan ; Khan, Afrasyab; Nazari, Marziyeh; Mirzaei, Hassan; Lup, Andrew Ng Kay; Baei, Mohammad Taghi; Chandiramouli, Ramanathan; Soltani, Alireza; Salehi, Aref; Javan, Masoud	Molecular Modeling and Simulation of glycine functionalized B12N12 and B16N16 nanoclusters as potential inhibitors of proinflammatory cytokines	Journal of Molecular Liquids	343	11749 4	41
2021	Shahini, N ; Ghasemzadeh, M; Javan, M ; Salimi, Z	Evaluation of the COVID-19 pandemic effect on the development of somatic symptoms in patients with mood disorders: a case-control study	New Microbes and New Infections	43	10091 7	9

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2022	Soltani, Alireza ; Khan, Afrasyab; Mirzaei, Hassan; Onaq, Marjan; Javan, Masoud ; Tavassoli, Samaneh; Mahmoodi, Nosrat O; Nia, Ali Arian; Yahyazadeh, Asieh; Salehi, Aref	Improvement of anti-inflammatory and anticancer activities of poly (lactic-co-glycolic acid)-sulfasalazine microparticle via density functional theory, molecular docking and ADMET analysis	Arabian Journal of Chemistry	15/1	10346 4	52
2022	Sun, Nabo ; Ansari, Mohammad Javed; Lup, Andrew Ng Kay; Javan, Masoud ; Soltani, Alireza; Khandoozi, Seyed Reza; Nia, Ali Arian; Tavassoli, Samaneh; Rahman, Md Lutfor; Sarjadi, Mohd Sani	Molecular docking and density functional theory simulation: Improved anti-inflammatory and anticancer properties of celecoxib using zinc oxide and	Arabian Journal of Chemistry	15/2	10356 8	38

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
		magnesium oxide nanoclusters				
2022	Sun, Nabo ; Ansari, Mohammad Javed; Lup, Andrew Ng Kay; Javan, Masoud ; Soltani, Alireza; Khandoozi, Seyed Reza; Nia, Ali Arian; Tavassoli, Samaneh; Rahman, Md Lutfor; Sarjadi, Mohd Sani	Improved anti-inflammatory and anticancer properties of celecoxib loaded zinc oxide and magnesium oxide nanoclusters: a molecular docking and density functional theory simulation	Arabian Journal of Chemistry	15/2	103568	-
2022	Majidinia, Reza; Javan, Masoud ; Ghazi, ME; Izadifard, Morteza	An ab initio DFT study of the optical and magnetic properties of Mn doped GaFeO ₃	Micro and Nanostructure s	165	207194	11

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2023	Zhang, Bin ; Wang, Hongzhi; Tazikeh-Lemeski, Elham; Javan, Masoud ; Gu, Juanfang; Soltani, Alireza; Guo, Linfeng	Comparative binding effects of celecoxib/poly (lactic-co-glycolic acid) microparticles with enhancing anti-inflammatory and anti-cancer activities: Density functional theory, molecular Docking, and ADMET calculations	Journal of Molecular Liquids	392	12333 2	29
2024	Javan, Masoud	Study of the electronic and optical properties of graphene-like ZnSe structure considering many body effects	Journal of Research on Many-body Systems	14/2	37-47	-

Year	Authors	Title	Journal	Volume/Issue	Pages	Citations
2025	Soleimani Fard, Mahbobeh ; Samadani Langeroodi, Narges; Javan, Masoud ; Dehno Khalaji, Aliakbar	The Removal of Methylene Blue from Aqueous Solutions Using CuFe ₂ O ₄ /PVP Nanocomposite: An Experimental and Theoretical Study	Iranian Journal of Soil and Water Research	55/11	2109-2124	-

Total Publications: 68+ | Total Citations: 1800+ | h-index: 28 | i10-index: 52

Research Impact Metrics

- **Total Publications:** 68+ peer-reviewed articles
- **Total Citations:** 1800+ (Google Scholar)
- **h-index:** 28
- **i10-index:** 52
- **Average Citations/Paper:** 26.5
- **Most Cited Paper:** "A DFT study on the interaction between 5-fluorouracil and B12N12 nanocluster" (2016) - **150+ citations**

Top Collaborators

1. **Prof. Alireza Soltani** (45+ joint publications)
 2. **Dr. Elham Tazikheh-Lemeski** (10+ joint publications)
 3. **Prof. Mohammad Taghi Baei** (8+ joint publications)
 4. **Dr. Nafiseh Abdolahi** (6+ joint publications)
-

Research Evolution

Phase 1 (2008-2013): Fundamental nanomaterials (Fullerenes, SiC nanocages)

Phase 2 (2014-2018): Functional materials for sensing and storage

Phase 3 (2019-2022): Biomedical applications (drug delivery, cancer therapy)

Phase 4 (2023-present): Integrated computational-experimental approaches

Technical Skills

Computational Software

- VASP, SIESTA, Gaussian, GAMESS, Quantum ESPRESSO
- Materials Studio, LAMMPS, GROMACS
- Python (NumPy, SciPy, Scikit-learn, TensorFlow)
- MATLAB, Mathematica

Programming Languages

- Python (Advanced)
- Fortran (Intermediate)
- C++ (Intermediate)
- Bash/Shell Scripting

Visualization Tools

- VESTA, VMD, PyMOL, Chimera
- OriginLab, Grace
- ParaView, VisIt