

Tabelle1

First Author	Journal	Year	DOI or Arxiv	AG González?	Interface	Topic
Marquetand	Faraday Discuss	2011	10.1039/C1FD00055A	Yes	--	LASER
Richter	JCTC	2011	10.1021/ct1007394	Yes	--	THEORY
Bajo	JPCA	2012	10.1021/jp208997r	Yes	--	LASER
Richter	JPCL	2012	10.1021/jp301312h	Yes	MOLPRO	cytosine
Mai	CPC	2013	10.1002/cphc.201300370	Yes	MOLPRO	cytosine
Corrales	PCCP	2014	10.1039/C3CP54677B	Yes	MOLPRO	different alkyl iodides
Gonzalez	Springer Series Chem.	2014	10.1007/978-3-319-02051-8_7	Yes	--	REVIEW
Mai	JCP	2014	10.1063/1.4875036	Yes	COLUMBUS	SO2
Richter	PCCP	2014	10.1039/C4CP04158E	Yes	MOLPRO	uracil
Crespo-Hernandez	JACS	2015	10.1021/ja512536c	Yes	MOLPRO	purine
Mai	IJCQ	2015	10.1002/qua.24891	Yes	--	THEORY
Martinez-Fernandez	JCTC	2015	10.1021/ct500909a	Yes	MOLCAS	cyclohexadieneendoperoxide
Banerjee	PCCP	2016	10.1039/C6CP03789E	No	MOLPRO	5-Phenyl-2H-tetrazole
Cao	CP	2016	10.1016/j.chemphys.2016.05.003	No	MOLPRO	oxazole
Mai	JPCL	2016	10.1021/acs.jpcllett.6b00616	Yes	MOLCAS	thiouracil
Mai	Nat Comm	2016	10.1038/ncomms13077	Yes	COLUMBUS	thiocytosine
Marazzi	JPCL	2016	10.1021/acs.jpcllett.5b02792	Yes	MOLCAS	benzophenon
Richter	JCTC	2016	10.1021/acs.jctc.6b00371	No	MOLPRO	uracil
Ruckebauer	JCP	2016	10.1063/1.4941948	Yes	only Wigner	
Andrew	JPCL	2017	10.1021/acs.jpcllett.7b01479	Yes	ADF	Rubipy
Bellshaw	CPL	2017	10.1016/j.cplett.2017.02.058	No	MOLPRO	CS2
Borin	PCCP	2017	10.1039/C6CP07919A	Yes	COLUMBUS	azacytosine
Mai	CP	2017	10.1016/j.chemphys.2016.10.003	Yes	MOLPRO	thymine
Mai	JCP	2017	10.1063/1.4999687	Yes	Turbomole	thiouracil
Murillo-Sánchez	CPL	2017	10.1016/j.cplett.2017.02.037	No	MOLPRO	CH2ICl
Peccati	Phil Trans R Soc A	2017	10.1098/rsta.2016.0202	Yes	COLUMBUS	bromouracil
Pederzoli	JCP	2017	10.1063/1.4978289	No	MOLPRO	thiophene, selenophene
Rauer	JACS	2017	10.1021/jacs.6b06701	Yes	MOLCAS	thymine 2
Schnappinger	PCCP	2017	10.1039/C7CP05061E	Yes	MOLCAS	thiophene
Siouri	JPCA	2017	10.1021/acs.jpca.7b03036	No	MOLPRO	6-thioguanine
Sun	JPCA	2017	10.1021/acs.jpca.6b12310	No	MOLPRO	2-phenylethyl-N,N-dimethylamine
Bellshaw	PCCP	2018	10.1039/C8CP05693E	No	MOLPRO	CS2
Cao	JMol Struct	2018	10.1016/j.molstruc.2017.11.008	No	MOLPRO (own interface)	thiazole
De Vetta	CPhotoC	2018	10.1002/cptc.201800169	Yes	Turbomole	BODIPY
Horton	PRA	2018	10.1103/PhysRevA.98.053416	Yes	MOLCAS	CH2I2
Li	JPCL	2018	10.1021/acs.jpcllett.8b00023	No	MOLPRO	Criegee intermediate
Mai	Molecules	2018	10.3390/molecules23112836	Yes	MOLCAS	Thiouracil
Menger	JCTC	2018	10.1021/acs.jctc.8b00763	Yes	Gaussian + Exciton	Exciton picture
Moreno-Armenta	CTC	2018	10.1016/j.comptc.2018.07.010	No	MOLPRO	C5Hn high spin
Murillo-Sánchez	PCCP	2018	10.1039/C8CP03600D	No	MOLPRO	CH2ICl and CH2BrI
Plasser	PCCP	2018	10.1039/C8CP05662E	Yes	LVC	SO2, nucleobases
Puglisi	PCCP	2018	10.1039/C7CP08026C	No	MOLPRO	Carbon hydride
Rauer	Monatshefte	2018	10.1007/s00706-017-2108-4	Yes	MOLPRO	Thymine dimer
Sandra	PCCP	2018	10.1039/C8CP07766E	Yes	MOLCAS	C2F2H2
Sapunar	CP	2018	10.1016/j.chemphys.2018.07.042	No	MOLCAS	Acetylacetone
Schnappinger	JCTC	2018	10.1021/acs.jctc.8b00492	Yes	ADF	dithiophene
Squibb	Nat Comm	2018	10.1038/s41467-017-02478-0	No	Turbomole, OpenMolcas	Acetylacetone
Zobel	CEJ	2018	10.1002/chem.201705854	Yes	ADF	Nitronaphthalene
Abedi	JPCL	2019	10.1021/acs.jpcllett.9b01522	No	OpenMOLCAS, GAUSSIAN	Dihydroazulene
Cao	PCCP	2019	10.1039/C8CP06891G	No	MOLCAS	disulfides
Frances-Monerris	ANIE	2019	10.1002/anie.201915656	No	openMOLCAS	Hg complexes
Ghosh	PCCP	2019	10.1039/C9CP00246D	No	MOLPRO	eumelanin monomer
Gomez	JPCA	2019	10.1021/acs.jpca.9b06103	Yes	LVC	SHARCgym
Gomez	PCCP	2019	10.1039/c8cp07766e	Yes	openMOLCAS	11DMFE
Heindl	CTC	2019	10.1016/j.comptc.2019.03.012	Yes	BAGEL	pyrrole
Horton	JCP	2019	10.1063/1.5086665	Yes	MOLCAS	CH2I2
Mai	JCTC	2019	10.1021/acs.jctc.9b00208	Yes	TURBOMOLE	2SeU
Mai	JCTC	2019	10.1021/acs.jctc.9b00282	Yes	multiple	CH2S
Mai	ChemSci	2019	10.1039/c9sc03671g	Yes	ADF	Re
Mignolet	JPCA	2019	10.1021/acs.jpca.9b00940	No	Analytical	Model
Nazari	PCCP	2019	10.1039/C9CP03147B	No	ADF	Phenanthrene
Plasser	JCTC	2019	10.1021/acs.jctc.9b00525	Yes	LVC	[Re(CO)3(phen)]+
Ruddock	SciAdv	2019	10.1126/sciadv.aax6625	No	MOLPRO	1,3-cyclohexene
Sangiogo Gil	PCCP	2019	10.1039/c9cp04313f	No	MOLCAS	triazoles

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Stankus	Nat Chem	2019	10.1038/s41557-019-0291-0	No	MOLPRO	N-methylmorpholine
Taffet	JPCB	2019	10.1021/acs.jpcc.9b04027	No	MOLCAS	carotinoids
Wang	JCTC	2019	10.1021/acs.jctc.9b00421	No	openMOLCAS	Quinazolinone
Wang	JCP	2019	10.1063/1.5116816	No	openMOLCAS	CH3I
Westermayr	ChemSci	2019	10.1039/c9sc01742a	Yes	Columbus / ML	CH2NH2+
Zhou	JPCL	2019	10.1021/acs.jpcclett.9b02747	No	MOLPRO	ethylene
Zobel	CphotoC	2019	10.1002/cptc.201900108	Yes	ADF	Nitro
Zobel	PCCP	2019	10.1039/C8CP03273D	Yes	ADF	Nitronaphthalene
Bokareva	PCCP	2020	10.1039/D0CP04781C	Yes	only Wigner	
Cao	PCCP	2020	10.1039/D0CP01450H	No	Gaussian	4TT, DTT
Chakraborty	Faraday Discuss	2020	10.1039/D0FD00110D	No	only kinetics fitting	
Chang	Nat Comm	2020	10.1038/s41467-020-17745-w	No	openMOLCAS	CH3I
Cho	JPCL	2020	10.1021/acs.jpcclett.0c00949	No	MOLPRO	Thiophenol
Frances-Monerris	ChemComm	2020	10.1039/D0CC01132K	No	ADF	Formyl-C, Formyl-U
Gong	CPL	2020	10.1016/j.cplett.2020.137506	No	MOLPRO	imine switches
Heim	JPCL	2020	10.1021/acs.jpcclett.9b03462	Yes	LVC / Turbomole	Acetone
Ibele	PCCP	2020	10.1039/d0cp01353f	No	MOLPRO	multiple
Ibele	JPCL	2020	10.1021/acs.jpcclett.0c02193	Yes	ORCA	polyadenine
Kochetov	JCP	2020	10.1063/5.0005940	No	only Wigner	
Lea	PCCP	2020	10.1039/D0CP01353F	No	MOLPRO, Gaussian	Ethylene, DMABN, fulvene
Li	ChinJCP	2020	10.1063/1674-0068/cjcp2006088	No	MOLPRO	Criegee intermediate
Liu	JCP	2020	10.1063/5.0026177	Yes	MOLCAS	CH2I2, CH2Br
Liu	PRX	2020	10.1103/PhysRevX.10.021016	Yes	MOLCAS	CH2I2
Mai	TCA	2020	10.1007/s00214-020-2555-6	Yes	LVC / ADF	Re protein
Norell	StructDyn	2020	10.1063/1.5143228	No	openMOLCAS	2-thiopyridone
Prjl	JPCL	2020	10.1021/acs.jpcclett.0c01439	No	BAGEL	volatile organics
Shu	JCTC	2020	10.1021/acs.jctc.0c00409	No	MOLPRO	Ethylene
Shu	JCTC	2020	10.1021/acs.jctc.0c00112	Yes	MOLPRO	Ethylene
Talotta	CEJ	2020	10.1002/chem.202000507	Yes	ADF	RuNO complex
Wang	JPCA	2020	10.1021/acs.jpca.0c03525	No	Gaussian	phenylhydrazon
Westermayr	JPCL	2020	10.1021/acs.jpcclett.0c00527	Yes	Schnarc	
Westermayr	JCP	2020	10.1063/5.0021915	Yes	SchNarc	
Zobel	Inorg Chem	2020	10.1021/acs.inorgchem.0c02147	Yes	LVC-ORCA	Fe complex
Abdelgawwad	Angew	2021	10.1002/anie.202111493	No	ORCA	o-Cobaltabis(dicarbollide) Anion
Araujo Valente	PCCP	2021	10.1039/D1CP03803F	No	BAGEL	Silole
Avagliano	JCTC	2021	10.1021/acs.jctc.1c00318	Yes	COBRAMM+MOLCAS	Acrolein in ACN
Carmona-Garcia	JACS	2021	10.1021/jacs.1c05149	No	openMOLCAS	HOSO
Carmona-Garcia	JACS	2021	10.1021/jacs.1c010153	No	openMOLCAS	HOSO2 and SO3
Chithra	PCCP	2021	10.1039/D1CP02587B	No	TURBOMOLE	2-mercaptobenzothiazole
Cox	JACS	2021	10.1021/jacs.1c01506	No	MOLCAS	hexafluorobenzene
Gessner	PCCP	2021	10.1039/D1CP03514B	Yes	only Wigner	triazacyclononane
Heindl	Inorg Chem	2021	10.1021/acs.inorgchem.0c03163	Yes	LVC-Gaussian	Ru SS
Heindl	JCP	2021	10.1063/5.0044807	Yes	LVC multiple	multiple
Heller	TCA	2021	10.1007/s00214-021-02741-0	No	MOLCAS	thiophene
Ibele	JCP	2021	10.1063/5.0045572	No	MOLPRO	cyclopropanone, fulvene, dithiane
Ibele	JCP	2021	10.1063/5.0071376	No	LVC	butatriene
Lee	Nat Comm	2021	10.1038/s41467-021-26193-z	No	ORCA	PAHs
Li	JCC	2021	10.1002/jcc.26783	No	openMOLCAS	cycl[3.3.3]azine
Losantos	PCCP	2021	10.1039/D1CP03617C	No	ORCA	Curcumin
Matsubaru	Bull Chem Soc Japan	2021	10.1246/bcsj.20210069	No	MOLCAS	butadiene
Murillo-Sánchez	New J. Phys	2021	10.1088/1367-2630/ac0c9b	No	MOLCAS	CH3I
Nag	JCP	2021	10.1063/5.0060934	No	Gaussian	3-hydroxyxochrome
Papai	PCCP	2021	10.1039/D1CP00771H	No	ORCA	trimethylamine Rydberg
Papai	Inorg Chem	2021	10.1021/acs.inorgchem.1c01838	No	ORCA	Fe NCH6
Pathak	Nat Chem	2021	10.1038/s41557-020-0507-3	No	MOLPRO	thiophene
Rott	StructDyn	2021	10.1063/4.0000102	No	MOLCAS	vinyl bromide
Sanchez	Nat Comm	2021	10.1038/s41467-021-21855-4	No	MOLCAS	OCS
Scutelnic	Nat Comm	2021	10.1038/s41467-021-25045-0	No	ORCA	pyrazine
Tamiya	PRResearch	2021	10.1103/PhysRevResearch.3.023244	No	own method (VQE)	model system
Vindel-Zandbergen	JCTC	2021	10.1021/acs.jctc.1c00346	No	MOLPRO	ethylene, methyleneimmonium, fulvene
Vinklarek	PCCP	2021	10.1039/D1CP01371H	No	only Wigner	
Weight	JCP	2021	10.1063/5.0061934	No	MOLPRO	ethylene, using modified SHARC
Wen	ChemRXiv	2021	10.33774/chemrxiv-2021-z3jhf	Yes	TURBOMOLE	molecular motor
Wernbacher	PCCP	2021	10.1039/D1CP02748D	Yes	only Wigner	
Yong	PNAS	2021	10.1073/pnas.2021714118	No	only Wigner	
Zhang	JCP	2021	10.1063/5.0037878	No	MOLCAS	CSH2
Zobel	ChemSci	2021	10.1039/D1SC02149D	Yes	LVC-ORCA	V complex
Zobel	Acc Chem Res	2021	10.1021/acs.accounts.1c00485	Yes	LVC	multiple
Avagliano	Phil Trans R Soc A	2022	10.1098/rsta.2020.0381	Yes	openMOLCAS	fulvene
Banerjee	Nat Comm	2022	10.1038/s41467-022-28997-z	No	ORCA	Fe(CO)5
Banerjee	Chem Eur J	2022	10.1002/chem.202200923	No	only Wigner	nitrate test
Bertram	PCCP	2022	10.1039/D2CP03167A	No	TURBOMOLE	2-thiooxazole
Calio	JCTC	2022	10.1021/acs.jctc.1c01048	No	openMOLCAS	CH2S
Endo	Front Chem	2022	10.3389/fchem.2022.859750	No	openMOLCAS	OCS2+
Esposito	PhC&PhB	2022	10.1111/php.13560	No	openMOLCAS	CH2OO and CH3CHOO
Frances-Monerris	Nat Comm	2022	10.1038/s41467-022-32170-x	No	OpenMOLCAS, GAUSSIAN	S2 and OSSO
Gabalski	JCP	2022	10.1063/5.0113079	No	MOLPRO	CS2
Ghosh	PCCP	2022	10.1039/D2CP00465H	No	MOLPRO	noncanonical nucleobase
Heindl	JPCL	2022	10.1021/acs.jpcclett.1c04143	Yes	LVC	Rubipy
Kilic	ACS ABM	2022	10.1021/acsabm.2c00202	No	only Wigner	Photodynamic therapy
Marsili	JPCA	2022	10.1021/acs.jpca.2c03783	No	BAGEL	2-hydroperoxypropanol
Matsubaru	PCCP	2022	10.1039/D2CP02418G	No	OpenMOLCAS and Bagel	Azobenzene / Diazocine
Messerly	CTC	2022	10.1016/j.comptc.2022.113634	No	openMOLCAS	HCCO+
Nag	JPCA	2022	10.1021/acs.jpca.2c04205	No	TURBOMOLE	3-mercaptopyran-4-one
Nag	JphPhA	2022	10.1016/j.jphotochem.2022.114024	No	Gaussian	Hydroxychromes
Nag	JphPhA	2022	10.1016/j.jphotochem.2021.113767	No	Gaussian	5-hydroxychrome
Papai	JCTC	2022	10.1021/acs.jctc.1c01184	No	ORCA	Fe NCH6
Ray	PCCP	2022	10.1039/D1CP05517H	No	Bagel and Gaussian	2-aminopurine
Razmus	PCCP	2022	10.1039/D2CP01268E	No	MOLPRO	CS2
Saiz-Lopez	Geophys Res Let	2022	10.1029/2022GL097953	No	openMOLCAS	Mercury in Stratosphere
Schnack-Petersen	JphPhA	2022	10.1016/j.jphotochem.2022.113869	No	ORCA	Azobenzene / Diazocine

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Schwinger	JACS	2022	10.1021/jacs.2c06683	No	ORCA	Aldehyd+BCI3
Shu	JCTC	2022	10.1021/acs.jctc.1c01080	No	MOLPRO	Ethylene
Valverde	JACS Au	2022	10.1021/jacsau.2c00250	Yes	TURBOMOLE	Se-Gua
Vindel-Zandbergen	JPCL	2022	10.1021/acs.jpcllett.1c04132	No	LVC	uracil
Wang	JPCA	2022	10.1021/acs.jpca.2c08025	No	only Wigner	Criegee intermediate
Wang	PCCP	2022	10.1039/D2CP01271E	No	Fitted PES	NH3
Westermayr	Nat Chem	2022	10.1038/s41557-022-00950-z	Yes	SchNarc	Tyrosine
Zederkof	JACS	2022	10.1021/jacs.2c04505	Yes	ORCA	Fe CNA bipy
Acheson	JCTC	2023	10.1021/acs.jctc.2c01113	No	MOLPRO	CS2
Arnanz	DyesPigments	2023	10.1016/j.dyepig.2023.111555	No	optimizer	azobenzenes
Arpa	CEJ	2023	10.1002/chem.202303191	No	optimizer	photogears
Arpa	Chem Meth	2023	10.1002/cmt.d.202200060	No	optimizer	photoswitches
Bertram	Faraday Discuss	2023	10.1039/D2FD00176D	No	Bagel	Cyclopentadienyl
Das	CEJ	2023	10.1002/chem.202302178	No	openMOLCAS	Ph-NN
Das	JmolLiQ	2023	10.1016/j.molliq.2023.121551	No	Gaussian	DMABN
Im	JPCA	2023	10.1021/acs.jpca.3c05280	No	openMOLCAS	ring opening
Jeong	PCCP	2023	10.1039/D3CP01169K	No	openMOLCAS	azaborine
Matsubaru	JPCA	2023	10.1021/acs.jpca.3c01669	No	Bagel	CH3X
Merritt	JCTC	2023	10.1021/acs.jctc.2c00968	No	openMOLCAS	multiple
Monari	PhotoPhotoSci	2023	10.1007/s43630-023-00431-3	No	ORCA	2-thienyl-3-hydroxychromone
Mu	Ultrafast Science	2023	10.34133/ultrafastscience.0015	No	Molpro	nucleobases
Nag	Chem Phys Impact	2023	10.1016/j.chphi.2023.100301	No	Gaussian	ESIPT
Nag	JPPA	2023	10.1016/j.jphotochem.2023.114538	No	TURBOMOLE	3HOX
Nag	JPPA	2023	10.1016/j.jphotochem.2023.115353	No	Gaussian	dihydroxychromone
Papai	JmatChemA	2023	10.1039/D3TA05985E	No	LVC	Fe(II) carbene
Polonius	JCTC	2023	10.1021/acs.jctc.3c00805	Yes	LVC/MM	CH2S
Prji	JPCA	2023	10.1021/acs.jpca.3c02333	No	Bagel	MeOOH
Reiner	JCTC	2023	10.1021/acs.jctc.2c01088	Yes	Analytical	NAFFS
Rozgonyi	Comm Chem	2023	10.1038/s42004-022-00796-z	No	LVC	Fe II complex
Santa Daria	PCCP	2023	10.1039/D3CP03656A	No	LVC create	PAHS
Schnack-Petersen	StructDyn	2023	10.1063/4.0000183	No	ORCA	4-(2-thienyl)-2,1,3-benzothiadiazole
Shu	JCTC	2023	10.1021/acs.jctc.2c01173	No	openMOLCAS	CH2S
Soydan	ACS Omega	2023	10.1021/acsomega.3c01226	No	only Wigner	tetraphenyls
Srut	JPCA	2023	10.1021/acs.jpca.3c04415	No	LVC	Creutz-Taube ion
Srut	PCCP	2023	10.1039/D2CP02981B	Yes	ORCA	Re complexes
Trabelsi	Astro&Astro	2023	10.1051/0004-6361/202245639	No	only Wigner	Mg molecules
Troß	JPCA	2023	10.1021/acs.jpca.3c01414	No	ORCA	acetyl iodide
Tsuru	JCTC	2023	10.1021/acs.jctc.2c01129	No	ORCA	Pyrazine + water
Vörös	JPCA	2023	10.1021/acs.jpca.3c02899	Yes	TURBOMOLE	nONA
Wada	JCC	2023	10.1002/jcc.27271	No	Molpro	MH2
Wen	JPCA	2023	10.1021/acs.jpca.3c05841	Yes	TURBOMOLE	Motor
Xie	PCCP	2023	10.1039/D3CP03730D	No	Gaussian	nucleobase PS
Xu	JPCA	2023	10.1021/acs.jpca.3c01036	No	only Wigner	motors
Zhao	JCTC	2023	10.1021/acs.jctc.2c01260	No	MOLPRO	NH3
Zhao	JCTC	2023	10.1021/acs.jctc.3c00813	No	openMOLCAS	several switches
Zhou	Nat Chem	2023	10.1038/s41557-023-01230-0	No	openMOLCAS	D2+D2
Zobel	Molecules	2023	10.3390/molecules28041668	Yes	LVC	Cr(dppd)2
Ariyageadsakul	JPCA	2024	10.1021/acs.jpca.4c04346	No	openMOLCAS	FHCl
Arpa	PCCP	2024	10.1039/D4CP00777H	No	ORCA	azaborine
Avanessian	JPCL	2024	10.1021/acs.jpcllett.4c02312	No	Model	NH3
Bokareva	Compre Comp Chem	2024	10.1016/B978-0-12-821978-2.00142-2	No	LVC	
Borne	Nat Chem	2024	10.1038/s41557-023-01420-w	No	openMOLCAS	quadracyclane
Cho	Nat Mat	2024	10.1038/s41563-024-01812-4	No	LVC create	OLEDs
Feng	Nat Chem	2024	10.1038/s41557-023-01410-y	No	openMOLCAS	DBO
Figueira Nunes	JACS	2024	10.1021/jacs.3c13046	No	Molpro	thiophenone
Franz	JACS	2024	10.1021/jacs.4c00548	Yes	LVC	Re S-S
Fushitani	JCP	2024	10.1063/5.0204769	No	ORCA	CH3I
Gallmetzer	JPCB	2024	10.1021/acs.jpbc.4c06924	Yes	Molpac-PI	Azo-Escitalopram
Hennefarth	JCTC	2024	10.1021/acs.jctc.4c01061	No	PySCF	azomethane
Hutton	JCP	2024	10.1063/5.0203667	No	OpenMolcas	MASH
Karak	JPCL	2024	10.1021/acs.jpcllett.4c01437	No	only Wigner	Singlet-triplet gaps
Kumar	JPCA	2024	10.1021/acs.jpca.4c03948	No	MOLPRO	Nitro-nucleobase
Li	ML: Sci Tech	2024	10.1088/2632-2153/ad4a04	No	MACE ML	
Lognon	ChemPhotoChem	2024	10.1002/cptc.202400078	No	ORCA	luminescent probe in water
Lopez-Pacios	JPCB	2024	10.1021/acs.jpbc.4c05179	No	optimizer	azobenzene deriv
Mannouch	JPCL	2024	10.1021/acs.jpcllett.4c00535	No	MOLPRO, Gaussian	MASH
Matsubara	ACS Earth	2024	10.1021/acsearthspacechem.4c00242	No	Gaussian	(CH4)2
Matsubaru	Bull Chem Soc Japan	2024	10.1093/bulcsj/uoae047	No	Gaussian	CH4, N2
Mausenberger	Chem Sci	2024	10.1039/D4SC04164J	Yes	Spainn	
Miron	JCTC	2024	10.1021/acs.jctc.4c01263	No	DFTB+	Motor
Nag	JPPA	2024	10.1016/j.jphotochem.2023.115353	No	Gaussian	3,5-dihydroxychromone
Pandey	JPCA	2024	10.1021/acs.jpca.4c02219	No	Gaussian	ESIPT
Pant	PRL	2024	10.1103/PhysRevLett.132.126903	No	Gaussian	TCNE trimer
Papineau	JPCL	2024	10.1021/acs.jpcllett.3c03014	No	Bagel Turbomole, ORCA	CH3NNCH3
Pengmei	SciData	2024	10.1038/s41597-024-03019-3	No	OpenMolcas	database
Peschel	PCCP	2024	10.1039/D4CP02492C	No	Fermions++	Enone-lewis acid
Pietruschka	ChemPhysChem	2024	10.1002/cphc.202400216	No	openMOLCAS	LiO2
Polonius	JCTC	2024	10.1021/acs.jctc.4c00169	Yes	LVC/MM	CH2S
Sami	JPCL	2024	10.1021/acs.jpcllett.4c00587	No	only Wigner	water clusters
Severino	Nat Photonics	2024	10.1038/s41566-024-01436-9	No	Gaussian	Furan
Shu	JCTC	2024	10.1021/acs.jctc.4c00424	No	theory only	theory only
Sun	JPCL	2024	10.1021/acs.jpcllett.4c02475	No	Turbomole	S8
Ulukan	PCCP	2024	10.1039/D4CP02474E	No	ORCA	dibenzofuran
Valverde	ACS AMI	2024	10.1021/acsami.4c04347	No	optimizer	Singlet-triplet gaps
Valverde	JCC	2024	10.1002/jcc.27521	No	ORCA	
Yang	PCCP	2024	10.1039/D4CP01085J	No	ORCA	CN
Zhou	JPCL	2024	10.1021/acs.jpcllett.3c03578	No	openMOLCAS	dioxetane
Zhou	Chin Phys B	2024	10.1088/1674-1056/ad0cc9	No	openMOLCAS	BrCN
Bachmair	PCCP	2025	10.1039/D4CP04834B	Yes	Analytical	NH3
Banerjee	Arxiv	2025	https://arxiv.org/abs/2502.14826	No	ORCA, Tinker	Cysteine
Ciborowski	JCC	2025	10.1002/jcc.70021	No	Molcas	Cr(CO)4bpy
Farkhutdinova	JPCA	2025	10.1021/acs.jpca.4c07472	Yes	ORCA, LVC	SO3, PtBr6, Rubpy3
Gudem	JPCA	2025	10.1021/acs.jpca.5c01912	No	openMOLCAS	NO2
Guo	JPCA	2025	10.1021/acs.jpca.4c08431	No	own interface (XMVB)	SN2 reaction
Jara-Cartes	JPCA	2025	10.1021/acs.jpca.4c08534	No	only Wigner	9-nitroanthracene
Ma	SciAdv	2025	10.1126/sciadv.adp9175	No	MOLPRO	cyclic disulfide
Papai	JCTC	2025	10.1021/acs.jctc.4c01331	No	LVC	Fe complexes
Restaino	JCP	2025	10.1063/5.0250153	No	ORCA	benzophenon
Robertson	CPL	2025	10.1016/j.cpllett.2025.142095	No	openMOLCAS	1,2-ditanene
Tiefenbacher	Digital Discovery	2025	10.1039/D5DD00044K	Yes	FieldSchnet	Furane
Vinod	Org. Chem. Front.	2025	10.1039/D4QO01832J	No	LVC	eumelanin
von Rhein	ChemComm	2025	10.1039/D4CC03943B	No	only Wigner	
Wang	ChemPhotoChem	2025	10.1002/cptc.202400418	No	optimizer	Diarylethenes
Zhou	JPCA	2025	10.1021/acs.jpca.4c04639	No	openMOLCAS	1,2-dioxetane
Zhou	JPCL	2025	10.1021/acs.jpcllett.5c00625	No	openMOLCAS	dimethyl-1,2-dioxetane