Available online at **www.joac.info**

ISSN: 2278-1862

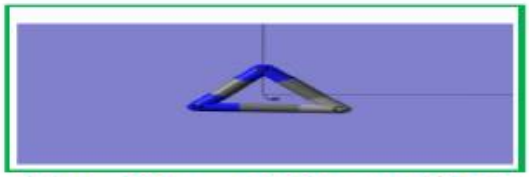
Journal of Applicable Chemistry

2022, 11 (4): 664-691

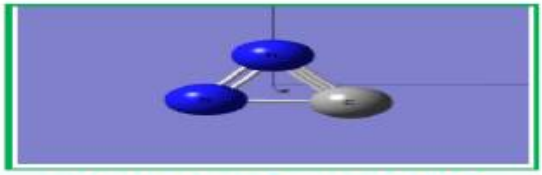
(International Peer Reviewed Journal)

New Chemistry News

$^{-}N=C=N^{-}$



New News of Chem (NNC)



ChemNewsNew (CNN)

CNN – 46

Aerogenbonds

Information Source	ACS.org ; sciencedirect.com
K. Somasekhara Rao, **Dept. of Chemistry,** **Acharya Nagarjuna Univ.,** **Dr. M.R.Appa Rao Campus,** **Nuzvid-521 201, India**	**R. Sambasiva Rao,** **School of Chemistry,** **Andhra University,** **Visakhapatnam 530 003, India**

Conspectus: Aerogen atoms ([AeA: [He Ne Ar, Kr, Xe Rn Og]) belong to 18th group of 18 column chemical elements periodic table. AeA or NgA exhibits Lewis's acid (LA) behaviour and forms complexes or adducts with Lewis bases (LB) including molecules or species with π electron systems. The aerogen (like triel, tetrel, pnic(t)ogen, chalcogen,halogen, hydrogen, spodium, regium) bond is also understood in terms of the σ-hole concept proposed by Politzer and Murray.

Knowledge based work-flows (with imbedded XI [:Artificial, eXplainable, Natural, Super Intelligence] , machine learning, deep learning, deep-NNs and preliminary-consciousness tools) have beentarget/focus of our investigations of speciation in different phases and environments evolving into better and better approachesin trans-disciplinary chemical sciences.

***Keywords*:**Interactions; Physics; Chemistry-Biology; Bonds; No-Bonds; Chemical bonds (CB); Electrovalent-B; Covalent Bond (CovB); Non-Covalent Chemical bonds (NCCB): [Nobel gas (aerogen), Halogen,Chalcogen, Pnicogen (or Pnictogen), Tetrel, Triel , Spodium, Regium (or

Coinage), alkali, alkaline earth, Hydrogen [{strong, weak}, dihydrogen, hydride]], Synthesis, spectroscopy, computational quantum chemistry, Molecular dynamics

	Layout	
I	Aerogen bonds in chemical systems	K(nowledge)Lab rsr.chem1979
II	Select Research Titles from ACS (American Chemical Society)	
III	Select Research Titles from SD (Science Direct)	

I. Aerogen bonds in chemical systems

Chemical bonds: The chemical bond, representing a lump of energy holding atoms of molecules together, is the central dogma of Chemical Sciences (CS). It playsthe role of a third eye in the rationalistic perception of material component of the Universe in Spatio-temporal frame. The conceptual understanding of the core of chemical bonding evolved with scientific progress and integration of all frameworks ---valence bond, advances in molecular orbital theories, static computationalquantum chemistry, molecular dynamics, spectroscopy up to atto-second scale etc---culminated into what exists today as the state-of-Knowledge-chemical bonding.

In the classical era, electrostatic and/or covalentinteractions were two pillars of formation/dissociation/ionization of molecular systems in solid, liquid, gaseous and solution phases. Although this approach accounted for more than major chunk of experimentalknowledge, deeper search continued to explain minor, but significant energetics/properties expressed by some systems and processes. Non-covalentinteractions were first enunciatedin 1983 by van der Waals [J.D. van der Waals, On the continuity of the gaseous and liquid state, Doctoral Dissertation, Leiden, the Netherlands, 1873]. Their relevance in life is unequivocally manifested in the double helixstructure of deoxyribonucleic acid[J.D. Watson, F.H.C. Crick, Molecular structure of nucleic acids: a structure for deoxyribose nucleic acid (DNA) Nature 171 (1953) 737–738].

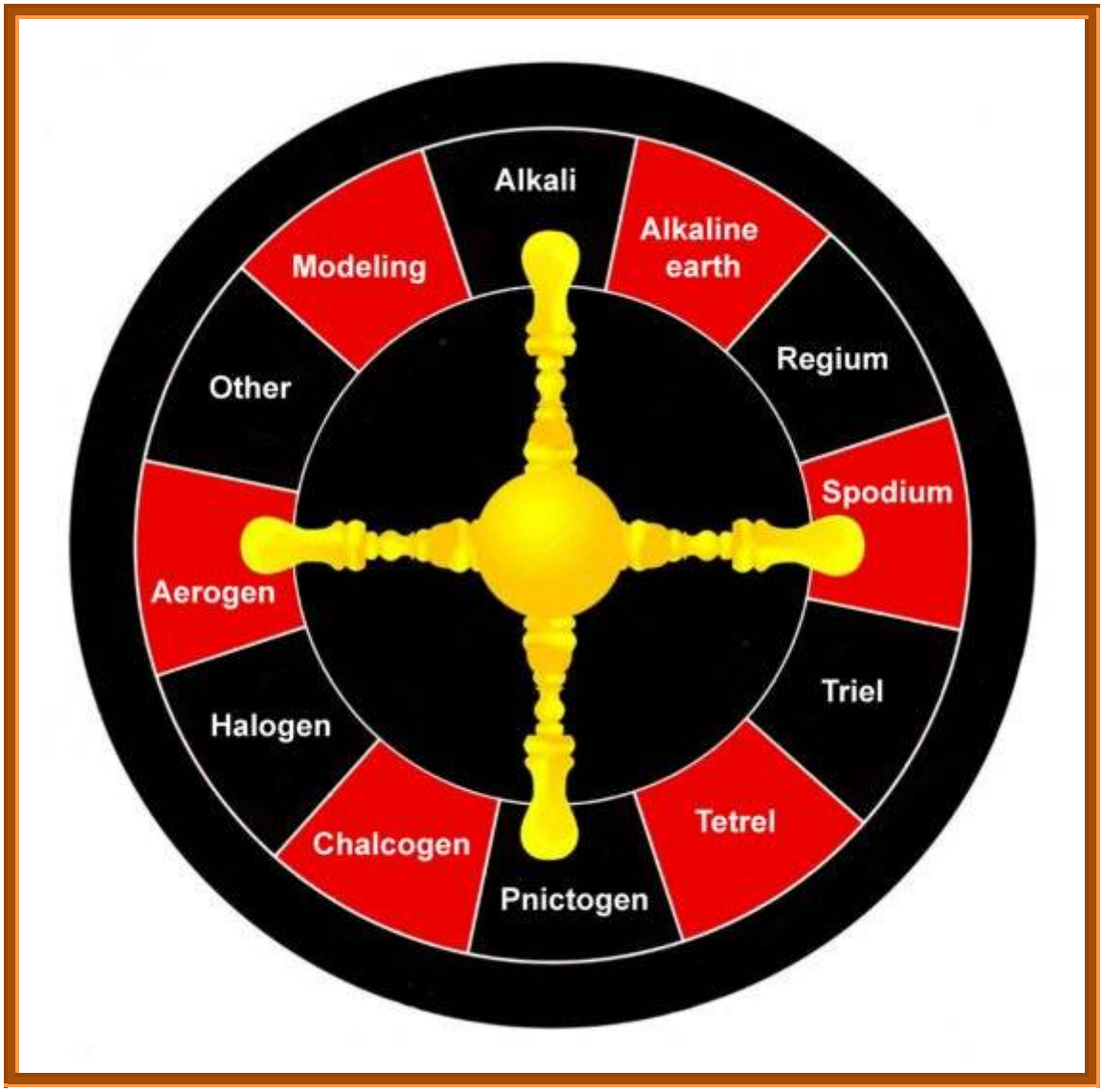
Animportant and foremost member of non-covalent bonds category is hydrogen bond. It was proposed a century ago and now indispensable in molecular chemistry, material science,crystalengineering, biology, protein-ligand (drug), protein-protein interactions etc.The outcome of researches in halogen bonding opened new vistas in apparent contradictory interactions. In the modern perceptive, these bonds are viewed as “Lewis acid-base”, “σ-hole – electron pair ” or “electron donor−acceptor (eDA)” interactions. A brief summary of spodium to aerogen bonds follow in a nutshell.

Column#	Abbrev	Abbrev	$$ bonds
	$$Bond	$$Atom	
1G	HB	HA	Hydrogen

18G	NgB	NgA	Nobel gas
	Or		
	AeB	AeA	Aerogen

An Aerogen bond is defined as an interaction between any electron donating moiety and an chemical element of group 18 group (NgA) acting as Lewis acid

Column#	Abbrev	Abbrev	$$ bonds
17G@	HaB	HaA	Halogen
16G@	ChB	ChA	Chalcogen
15G	PnB	PnA	Pnicogen or Pnictogen
14G	TtB	TtA	Tetrel
13G	TrB	TrA	Triel
12G	SPB	SPA	Spodium
11G	CiB or RgB	CiA or RgA	Coinage or Regium
2G	AEB AlkEarB	AEB AlkEarA	Alkaline-Earth
1G	AkB AlkB	AkA AlkA	Alkali



Aerogen bonds

Aerogenbond (AeB) or

Noble gas bond (NgB)

- ☞ Is a member of set (or family) of σ_hole (or simply σ) bonds
- ☞ σ-hole on theaerogen atom is located approximately on the extension of the covalent bonds to this atom

Def: Non-covalent bond arising due to interaction between

- ✓ a covalently-bonded Group-18 (noble gas or aerogen) atom (NgA or AeA) functioning as Lewis acid (or an electron-acceptor) andelectron donor playing the role of Lewis base

	🔔 Lewis acid property of aerogen atoms arise due to existence of an electron-deficient region (called σ-hole) 🔔 σ-hole is distributed on the outermost portion of these aerogen atoms 🔔 σ-hole region characterized by a positive molecular electrostatic potential (MESP)
	✓ Very much like those of the halogen bond because of the similar misshaped electron clouds of the halogen atom

Characteristics of Aerogenbond	AeBs exhibit 🔔 Less directionality than other σ-hole interactions like halogen bonds
	Directional tunability → Great promise to fabricate ! Smart molecules and materials with o Desired functions, properties
Electrondonors inaerogen bonds	o Lone pairs from molecules like o NH3 or NCH o Pi electrons o Single electron donors o Radical species o Metal hydrides ✓ Negative site on the Lewis base is responsible for formation and directionality of aerogenbonds
Strength of AeB	✓ Increases as size of the aerogen atom increases {He to Rn} ✓ Increases by cooperative effects
	Generally comparable with 🔔 Lone pair–aerogen interaction 🔔 conventional hydrogen bonds 🔔 Very much like those of the halogen bond because of the similarmisshaped electron clouds of the chalcogen atom andhalogen atom
	Depends upon ! Characteristics of aerogen atom ! Nature of the electron-donor ! Substituent effects on the Lewis acid / Lewis base ! Cooperativity with other intermolecular interactions 🔔 Cooperative synergetic or effects Between types of intermolecular interaction

Components of Non-covalent (Aerogen) Interactions	☞ Electrostatic effects ☞ Charge-transfer from the bonding orbital in the Lewis base to the antibonding orbital of the Lewis acid ☞ Polarization ☞ Dispersion ☞ Cooperative effects
Applications in molecular design	Functions as a molecularlinker in ☞ Molecular recognition (MR) ☞ Material synthesis (MS) ☞ Structureformation, dynamics ☞ Chemical reactions
Aerogen bond formation detected by	☞ Bond-length change ☞ Interaction energy ☞ Topological property ☞ Electron charge density and its Laplacian ☞ Charge transfer
Expt. evidence for Aerogen bond	Crystal structure experiments ☞ Agreement with the theoretical/computational results ☞ Existence of the aerogen bond (AFM) ☞ Protein Data Bank ☞ Crystal packing processes
Critical role in	🔔 Protein folding 🔔 Stacking of nucleobases 🔔 Drug binding 🔔 Self-assembly

Single-electron Non_Cov bonds

single-electron hydrogen bond Se HB	CH3···HCN CH3···H2O CH3···NH3	Methyl radical electron acts as the proton acceptor
single-electron tetrel bond SE. TtB	FXH3···CH3 (X = C, Si, Ge, and Sn) complexes	
single-electron σ-holebond SE.SigB	σ-hole region of Group 14-17 atoms	unpaired electron of the methyl radical

single-electron aerogen bond SE.AeB	KrOF2, KrO3, XeOF2 and XeO3	methyl (CH3) or ethyl (C2H5) radical
	Probes ✓ Molecular electrostatic potential ✓ Quantum theory of atom in molecules ✓ Natural bonding orbital ✓ Noncovalent interaction index analyses	
	Information bit: o Formation of an O···H interaction increase the strength of the SEAB, when they coexist in a ternary complex	

Cooperativity effect

Cooperativity effect	Cumulative strength of (two or moreor networks of) noncovalent bondsis larger or smaller (when they work in concert)compared to sum of the individual bondstrengths
Mechanism of Cooperativity	! The formation of first noncovalent bond results in a change in electron distribution of monomers ! This happens in such a way that an electron donating site nearby the electron acceptor site becomes ! potentially a better electron donor ! Cooperatively forms a second noncovalent bond. Similarly, the nearby electron-accepting sites become less prone for a second interaction
Responsible factors for co-operativity	✓ Many body interactions ✓ Secondary interactions ✓ Conformation changes ✓ Chelate effect
Cooperativity ofhydrogen bonds	Historical : In water complexes in 1957 Recent: 1970-2022

Cooperativity effect in non-cov_interactions (aerogen bond + another NCB)

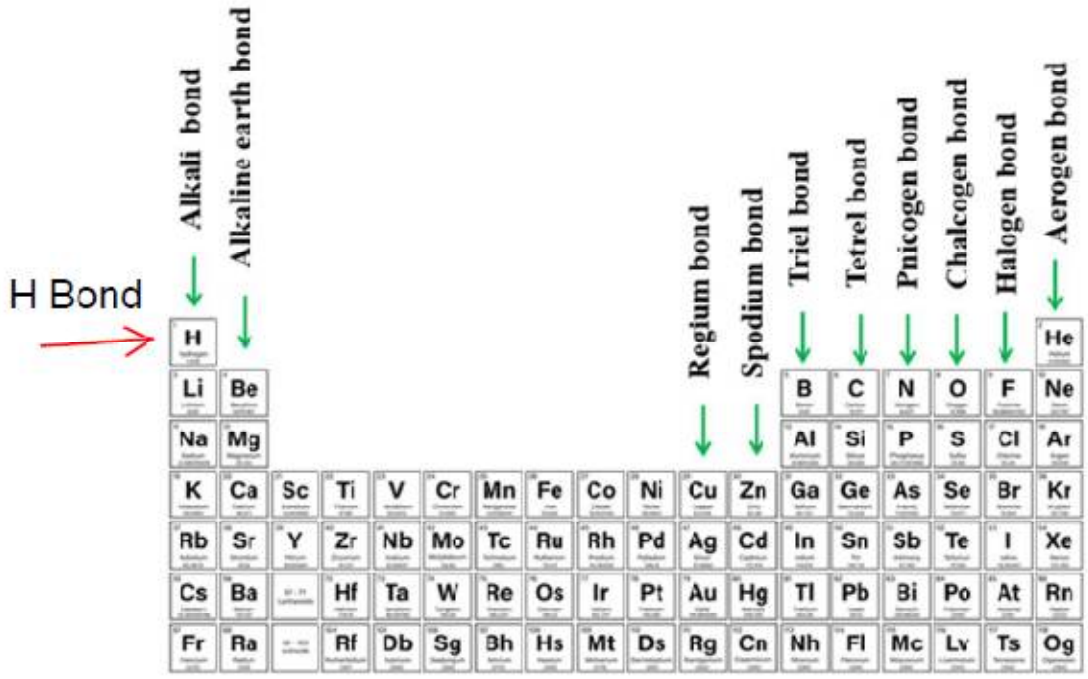
Example 1: Aerogen-bonding interaction increases in the presence ofan anion-π or a lone pair-π interaction.The estimated cooperativeenergies are between −0.27 and −11.96 kcal/mol
Example 2:In aerogen-π and cation-πinteractions, induction effects areresponsible for the stabilization

of these species besidesthe dispersion forces

Example 3: Aerogen bond and a hydrogen- or lithium-bonding interactionoriginated

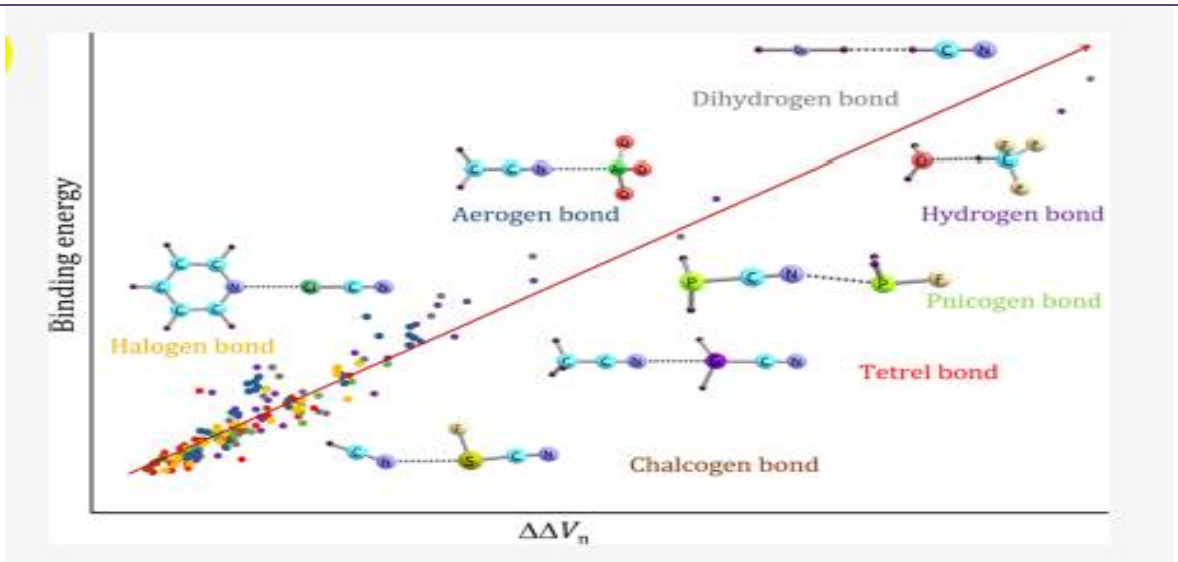
by the charge transfer and electrostatic effects betweenthe interacting monomers

Chem Systems: O3Z···NCM···NCX (Z = Ar, Kr, Xe; M = H, Li;X = H, F, and CH3) complexes



NonCovalent-Bonds
Sigma- pi- Interactions

NonCov-Bond	☞ **[HyB DHyB** ☞ **TrB TtB PtB** ☞ **ChB, HaB NgB]**	NgB.	ACS.	**03**



II. *Select Research Titles from American Chemical Society Journals*

Aeroogen Bond	NgB.	ACS.	**01**

Comp Quan Chem (CQC)	
LA	**LB**
AeOF2 (Ae = Kr, Xe)	o Diazines o Pyridazine, Pyrimidine, o Pyrazine

Software	Gaussian 03 MOLPRO 2012
Tasks	Geom opt Frequency computations
Interaction energies	Corrected for BSSE by standard counterpoise procedure

Theory level	MP2		
Basis sets	aug-cc-pVDZ-PP	Xe	To incorporate relativistic effects
	aug-cc-pVDZ	other atoms	

Probe		Software	Inf
Energy decomposition analysis	EDA	ADF modeling suite	BLYP/ZORA/TZ2P level
Molecular Electrostatic potentials	MEPs	WFA-SAS	MP2/aug-cc-pVDZ level
NBO analysis	NBO	NBO	
Noncovalent interaction index	NCI	MultiWFN	MP2/aug-cc-pVDZ level

Descriptors		
Bond critical properties	Electron density	ρ
	Laplacian of electron density	$\nabla^2\rho$
	Total electron energy	H kcal mol-1
Second-order NBO perturbation energies (E2)	For for charge transfer between indicatedorbitals in σ-hole bonded F2OAe (Ae = Kr, Xe) complexes Ex: LP(N1)→σ*AeO	
EDA	Total DFT-D interaction energy of σ-complexes→ ✓ Pauli repulsion (EPauli) + ✓ Electrostatic (Eelstat) + ✓ orbital interaction (Eoi)+ dispersion (Edisp)	

Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a N···N Pnicogen Bond	J. Phys. Chem. A, 2021, 125, 2, 657–668 Doi.org/10.1021/acs.jpca.0c10814		
Mariusz Michalczyk, Magdalena Malik, Wiktor Zierkiewicz			
	NgB.	ACS.	01

Dissection of the Origin of π-Holes and the Noncovalent Bonds in Which They Engage	J Phys. Chem A, 2021, 125, 30, 6514-6528 DOI: 10.1021/acs.jpca.1c05431		
Steve Scheiner			
	NgB.	ACS.	02

Molecular Electrostatic Potential Reorganization Theory to Describe Positive Cooperativity in Noncovalent Trimer Complexes	J. Phys. Chem. A, 2020, 124, 11, 2231-2241 DOI: 10.1021/acs.jpca.9b11538		
Padinjare Veetil Bijina and Cherumuttathu H. Suresh			
	NgB.	ACS.	03

Hydrophobic Solvation of Gases (CO2, CH4, H2, Noble Gases) in Clay Interlayer Nanopores	J. Phys. Chem. C, 2017, 121, 47, 26539-6550 DOI: 10.1021/acs.jpcc.7b09768
Greeshma Gadikota, Baptiste Dazas, Gernot Rother, Michael C. Cheshire and Ian C. Bourg	
	NgB. ACS. 04

Noble gas Bonding

NgB. ACS. **05**

Comp Quan Chem (CQC)

NgMX	Ng = He, Ne, Ar, Kr, Xe, Rn; M = Cu, Ag, Au; X = F,Cl, Br, I

Software	Gaussian 03	
Bonding analyses	☞ Natural Bond Orbital (NBO) ☞ Natural Resonance Theory (NRT)	GENNBO 6.0W

Theory level	Coupled-cluster CCSD(T)			
Basis sets	Convergent triple-ζ basis sets	aug-cc-pVTZ-PP	Include small-core energy-consistent relativistic pseudopotentials (PP) to account for relativistic effects	☞ Xe, Rn, I
	Systematically augmented correlation-consistent triple-ζ Dunning basis sets		aug-cc-pVTZ	☞ Other atoms

Insight into the Bonding Mechanism and the Bonding Covalency in Noble Gas–Noble Metal Halides: An NBO/NRT Investigation	J. Phys. Chem. A, 2017, 121, 27, 5183-5189 DOI: 10.1021/acs.jpca.7b02047
Guiqiu Zhang, Lei Fu, Hong Li, Xuchan Fan and Dezhan Chen	
	NgB. ACS. 05

How to Twist, Split and Warp a σ-Hole with Hypervalent Halogens	J. Phys. Chem. A, 2016, 120, 47, 9431-9445 DOI: 10.1021/acs.jpca.6b07894
Omer Kirshenboim and Sebastian Kozuch	
	NgB. ACS. 06

Noble gas Bonding

NgB. ACS. **07**

Comp Quan Chem (CQC)

AuNgX	Ng = Ar, Kr, Xe; X = F, Cl,Br, I

Software	Gaussian 09
Tasks	Geom opt Frequency computations

Theory level	MP2 DFT(B3LYP) DFT(M062X)
Basis sets	Def2-TZVPPD

Probe		Software
Topological analysis of the ρ(r)	wave function approximated by the CCSD method with the Def2-TZVPPD basisset.	AIMAll
Single-point Energy	o DFT(B3LYP) + o Relativistic effects described by the zero-order regular approximation (ZORA) o Basis set : optimized Slater-type ,	ADF program

Nature of the Bonding in the AuNgX (Ng = Ar, Kr, Xe; X = F, Cl, Br, I) Molecules. Topological Study on Electron Density and the Electron Localization Function (ELF)	J. Phys. Chem. A, 2015, 119, 11, 2401-2412 DOI: 10.1021/jp508266k		
Emilia Makarewicz, Agnieszka J. Gordon and Slawomir Berski			
	NgB.	ACS.	07
Noble Gas Adsorption in Metal–Organic Frameworks Containing Open Metal Sites	J. Phys. Chem. C, 2014, 118, 22, 11685-11698 DOI: 10.1021/jp501495f		
John J. Perry, Stephanie L. Teich-McGoldrick, Scott T. Meek, Jeffery A. Greathouse, Maciej Haranczyk and Mark D. Allendorf			
	NgB.	ACS.	08

Noble gas Bonding	NgB.	ACS.	**09**

Comp Quan Chem (CQC)	
HNgFNgH+	Ng = He-Xe

Software	Gaussian 03	
Tasks	Geom opt Frequency computations	
	Intrinsic reaction coordinate (IRC) o MP2 and DFT(B3LYP) levels of theory	To unambiguously relate any TS to its interconnected energyminima

	☞ Atomic charges computed by	☞ NBO analysis o MP2/aug-cc-pVTZ/SDD wave function
	☞ Chemical bonding analysis	☞ Theory of atoms-in-molecules (AIM) o MP2/aug-cc-pVTZ/SDD electron density ☞ Software : AIM2000,
	☞ AIM analysis -- Attractor interaction—Bonding properties	☞ Charge density ☞ Laplacian of the charge density ☞ Energy density H at the bond critical points

Theory level	Ab-initio MP2	
Basis sets	Dunning's correlation consistent double- and triple-_ basis sets, augmented with diffuse functions (aug-cc-pVDZand aug-cc-pVTZ)	H, F, He, Ne, Ar, and Kr
	RelativisticStuttgart/Dresden (SDD) effective core potential and the valencebasis set designed for this ECP	Xe

	Probe	Software
Topological analysis of the ρ(r)	Wave function approximatedby the CCSD method with the Def2-TZVPPD basisset	AIMAll
Single-point Energy	o DFT(B3LYP) + o Relativistic effects described by the zero-order regular approximation (ZORA) o Basis set : optimized Slater-type ,	ADF program

Cationic Noble Gas Hydrides: A Theoretical Investigation of Dinuclear HNgFNgH+ (Ng = He−Xe)	J. Phys. Chem. A, 2010, 114, 27, 7382-7390 DOI: 10.1021/jp102018n			
Stefano Borocci, Nicoletta Bronzolino, Maria Giordani and Felice Grandinetti				
		NgB.	ACS.	09

Molecular Dynamics Simulations of Deuterium Trapping and Re-emission in Tungsten Carbide	J. Phys. Chem. C, 2010, 114, 12, 5382-5390 DOI: 10.1021/jp9054473			
Katharina Vörtler and Kai Nordlund				
		NgB.	ACS.	10

List of Publications of Vincenzo Aquilanti	J. Phys. Chem. A, 2009, 113, 52, 14193-14205 DOI: 10.1021/jp9097777			
Vincenzo Aquilanti				
		NgB.	ACS.	11

Noble Gas Anions: A Theoretical Investigation of FNgBN- (Ng = He−Xe)	J. Phys. Chem. A, 2007, 111, 40, 10144-10151 DOI: 10.1021/jp0743673
Paola Antoniotti, Stefano Borocci, Nicoletta Bronzolino, Patrizio Cecchi and Felice Grandinetti	
NgB. ACS. 12	

Determination of branching ratio and collisional mixing rate of potassium (52PJ) doublets following 193-nm photodissociation of potassium iodide in the presence of argon, helium, methane, and carbon dioxide	J. Phys. Chem., 1993, 97, 3, 604-609 DOI: 10.1021/j100105a012
Ching Bin Ke, Shiow Hwa Chou, King Chuen Lin and Wei Tzou Luh	
NgB. ACS. 13	

Collisional quenching of electronically excited tin atoms, Sn(5p2 3P1) and Sn(5p2 3P2), by time-resolved attenuation of atomic resonance radiation	J. Phys. Chem., 1976, 80, 2, 91-97 DOI: 10.1021/j100543a001
P. D. Foo, J. R. Wiesenfeld, M. J. Yuen and D. Husain	
NgB. ACS. 14	

Xenon in Rigid Oxide Frameworks: Structure, Bonding and ExplosiveProperties of Layered Perovskite K4Xe3O12	J. Am. Chem. Soc.,2016, 138, 13838−13841 DOI: 10.1021/jacs.6b09056
Sergey N. Britvin, Sergei A. Kashtanov, Sergey V. Krivovichev and Nikita V. Chukanov	
NgB. ACS. 15	

Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons	Molecules, 2021, 26, 1740. doi.org/10.3390/molecules26061740
Wiktor Zierkiewicz, Mariusz Michalczyk and Steve Scheiner	
NgB. ACS. 16	

How to Twist, Split and Warp a #-Hole with Hypervalent Halogens	J Phys Chem., 2016, 120(47):9431-9445 doi: 10.1021/acs.jpca.6b07894
Omer Kirshenboim, and Sebastian Kozuch	
NgB. ACS. 17	

Structure and Stability of the Organo-Noble Gas Molecules XNgCCX and XNgCCNgX (Ng = Kr, Ar; X = F, Cl)	J. Phys. Chem. A, 2007, 111, 44, 11261-11268 DOI: 10.1021/jp071242p
Scott Yockel, Evan Gawlik and Angela K. Wilson	
NgB. ACS. 18	

Endohedral energies and translation of fullerene-noble gas clusters G@Cn (G = helium, neon, argon, krypton and xenon; n = 60 and 70)	J. Phys. Chem., 1993, 97, 33, 8562-8563 DOI: 10.1021/j100135a005
L. Pang and F. Brisse	
NgB. ACS. 19	

Surface assisted xenon-xenon bonding?	J. Phys. Chem., 1991, 95, 10, 4033-4037 DOI: 10.1021/j100163a028
Roald Hoffmann, Meinolf Kersting and Zafiria Nomikou	
NgB. ACS. 20	

Complexes of XeHXe+ with Simple Ligands: A Theoretical Investigation on (XeHXe+)L (L = N2, CO, H2O, NH3)	J. Phys. Chem. A, 2015, 119, 11, 2383–2392doi.org/10.1021/jp5075835
Stefano Borocci, Maria Giordani, and Felice Grandinetti	
NgB. ACS. 21	

III. Select Research Titles from Science Direct

An efficient error-correction model to investigate the rotational structure and microwave spectrum of Ar–AgF complex	Chemical Physics, 18 April 2022, 111545 doi.org/10.1016/j.chemphys.2022.111545
Yanshan Tian, Tong Cheng, Rui Zheng	
NgB. SD. 01	

Spodium bonds and metal–halogen···halogen–metal interactions in propagation of monomeric units to dimeric or polymeric architectures	Journal of Moleculadr Structure, Volume 1252, 15 March 2022, 132144 doi.org/10.1016/j.molstruc.2021.132144
Vali Alizadeh, Ghodrat Mahmoudi, Damir A. Safin	
NgB. SD. 02	

From LAr to L-ArBeO (L = He, Ne, Ar, HF): Switching on σ-hole effects in non-covalent interactions	Chemical Physics Letters, 768, April 2021, 138402 doi.org/10.1016/j.cplett.2021.138402
Borocci, Stefano Felice Grandinetti, Nico Sanna	
NgB. SD. 03	

Chapter 4: A combined theoretical and CSD perspective on σ-hole interactions with tetrels, pnictogens, chalcogens, halogens, and noble gases	Hot Topics in Crystal Engineering, 2021,Pages 119-155 doi.org/10.1016/B978-0-12-818192-8.00001-9
Rosa M. Gomila Tiddo J. Mooibroek Antonio Frontera	
NgB. SD. 04	

Chapter 2: The intermolecular chemical bond: Physical facts and geometric fiction	Theoretical and Computational Chemistry, 20, 2021, Pages 25-52 doi.org/10.1016/B978-0-12-823747-2.00002-0
Angelo Gavezzotti	
NgB. SD. 05	

Chapter One: Recent advances in NMR crystallography and polymorphism	Annual Reports on NMR Spectroscopy, Volume 102, 2021, Pages 1-80 doi.org/10.1016/bs.arnmr.2020.10.001
Scott A. Southern, David L. Bryce	
NgB. SD. 06	

Chapter One: Indirect spin-spin coupling constants across noncovalent bonds	Annual Reports on NMR Spectroscopy, Volume 104, 2021, Pages 1-73 doi.org/10.1016/bs.arnmr.2021.05.002
Jarosław Jaźwiński	
NgB. SD. 07	

Pentavalent P…π phosphorus bonding with associated Cl…π halogen bonding in influencing the geometry of POCl3-Phenylacetylene heterodimers: Evidence from matrix isolation infrared spectroscopy and ab initio computations	Journal of Molecular Structure, Volume 1224, 15 January 2021, 129288 doi.org/10.1016/j.molstruc.2020.129288
B. Suryaprasad, Swaroop Chandra, K. Sundararajan	
NgB. SD. 08	

The interplay and the formation of σ-hole in the π···LiX and pseudo-π···LiX (X = F, Cl and CN) lithium bonds involving unsaturated and homocyclic hydrocarbons	Computational and Theoretical Chemistry, Volume 1186, 15 September 2020, 112899 /doi.org/10.1016/j.comptc.2020.112899
D. G. Rego, B. G. Oliveira	
NgB. SD. 09	

C(sp3) atoms as tetrel bond donors: A crystallographic survey	Coordination Chemistry Reviews, Volume 413, 15 June 2020, 213265 doi.org/10.1016/j.ccr.2020.213265
Andrea Daolio, Patrick Scilabra, Giuseppe Resnati	

	NgB.	SD.	10

Halogen bond in separation science: A critical analysis across experimental and theoretical results	Journal of Chromatography A, Volume 1616, 12 April 2020, 460788 doi.org/10.1016/j.chroma.2019.460788
Paola Peluso, Victor Mamane, Sergio Cossu	

	NgB.	SD.	11

σ/π-Hole noble gas bonding interactions: Insights from theory and experiment	Coordination Chemistry Reviews, Volume 404, 1 February 2020, 213112 doi.org/10.1016/j.ccr.2019.213112
Antonio Bauzá, Antonio Frontera	

	NgB.	SD.	12

Tetrel bonding interactions at work: Impact on tin and lead coordination compounds	Coordination Chemistry Reviews, Volume 384, 1 April 2019, Pages 107-125 doi.org/10.1016/j.ccr.2019.01.003
Antonio Bauzá, Saikat Kumar Seth, Antonio Frontera	

	NgB.	SD.	13

Tetrel bonding on graphene	Computational and Theoretical Chemistry, 1147, 1 January 2019, Pages 8-12 doi.org/10.1016/j.comptc.2018.11.011
Yu Zhang, Weizhou Wang, Yi-Bo Wang	

	NgB.	SD.	14

Sigma-Hole Interactions in Anion Recognition	Chem, 4, Issue 4, 2018, Pages 731-783 doi.org/10.1016/j.chempr.2018.02.022
Jason Y. C. Lim, Paul D. Beer	

	NgB.	SD.	15

A computational study on the strength and nature of bifurcated aerogen bonds	Chemical Physics Letters, 698, 16, Pages 1-6 doi.org/10.1016/j.cplett.2018.02.066
Mehdi D. Esrafili, Asma Sadr-Mousavi	

	NgB.	SD.	16

Anionic tetrel bonds: An ab initio study	Chemical Physics Letters, 691, January 2018, Pages 394-400 doi.org/10.1016/j.cplett.2017.11.051
Mehdi D. Esrafili, Soheila Asadollahi, Parisasadat Mousavian	

	NgB.	SD.	17

Fluorinated elements of Group 15 as pnictogen bond donor sites	Journal of Fluorine Chemistry, 203, November 2017, Pages 62-74 doi.org/10.1016/j.jfluchem.2017.10.002
Patrick Scilabra, Giancarlo Terraneo, Giuseppe Resnati	
	NgB. SD. 18

A theoretical survey of substituent effects on the properties of pnicogen and hydrogen bonds in cationic complexes of PH4+ with substituted benzonitrile	Journal of Molecular Graphics and Modelling, 77, October 2017, Pages 64-71 doi.org/10.1016/j.jmgm.2017.08.010
Sotoodeh Bagheri, Hamid Reza Masoodi, Ali Reza Akrami-Mohajeri	
	NgB. SD. 19

{{{{{{{

Prediction of neutral noble gas compounds LiNgF (Ng=Kr, Xe and Rn)	Computational and Theoretical Chemistry, 1113, 1 August 2017, Pages 8-13 doi.org/10.1016/j.comptc.2017.04.011
Rui Zhao, Li Sheng, Kunqi Gao	
	NgB. SD. 20

Aeroogen Bond	NgB.	SD	**20**

Comp Quan Chem (CQC)	
species	
LiNgF Decomposition	o Ng = [Xe Rn]

Comp Quan Chem (CQC)		
CQC	Software	Gaussian 03
Geom opt frequency computations	DFT (B3LYP) MP2 CCSD(T)	Theory level
	aug-cc-PVTZ (AVTZ) Dunning's correlation consistent triple-zeta basis sets with diffuse functions	F, Li and Kr atoms
	valence basis set + aug-cc-PVTZ-PP relativistic effective core pseudopotentials (ECPs)	Xe and Rn atoms
Minimum energy paths of unimolecular decomposition	intrinsic reaction coordinate (IRC) c	B3LYP MP2
Bond nature of the LiNgF species	Natural bond orbital (NBO) analysis QTAIM topological analysis	

MP2 energies	AVTZ aug-cc-PVQZ (AVQZ) basis sets

CCSD(T)	AVTZbasis set
CCSD(T)/AVQZ energies	$E^{CCSD(T)/aug-cc-pvqz} = E^{MP2/aug-cc-pvqz} + \Delta_{MP2}^{CCSD(T)}$ $\Delta_{MP2}^{CCSD(T)} = E^{CCSD(T)/aug-cc-pvtz} + E^{MP2/aug-cc-pvtz}$
CCSD(T)/CBS energies	Two-point extrapolation formula $E_{CBS} = \frac{X^3E(X) - (X-1)^3E(X-1)}{X^3 - (X-1)^3} \quad (X = 4)$

Probes	Inference	Sub-hypotheses
Bond lengths	✓ LiANg bond lengths < Rcov(LiANg) ✓ calculated NgAF bond lengths are in the range from Rcov(NgAF) to RvdW(NgAF).	➔ LiAXe bond is electrostatic ➔ XeAF, LiARn and RnAF bonds is weak interaction with some covalent property
NBO analysis	✓ LiNgF species large electrons transferred from LiNg fragment to F atom.	
QTAIM parameters	✓ Low q(rc), ✓ Positive r2q(rc), ✓ Small |H(rc)| and G(rc)/q(rc) suggest that the ,	

}}}}}

Helium Shows New Chemistry Not Seen Anywhere Else	Chem, 2, Issue 4, 13 April 2017, Pages 466-467 doi.org/10.1016/j.chempr.2017.03.008		
Jorge Botana, Mao-sheng Miao			
	NgB.	SD.	21

Importance of Nonclassical σ Hole Interactions for the Reactivity of λ3 Iodane Complexes	The Journal of Organic Chemistry, 82, Issue 22, 2017, Pages 11799-11805 doi.org/10.1021/acs.joc.7b01716		
Halua Pinto de Magalhães, Antonio Togni, Hans Peter Lüthi			
	NgB.	SD.	22

An ab initio study on anionic aerogen bonds	Chemical Physics Letters, 667, January 2017, Pages 337-344 doi.org/10.1016/j.cplett.2016.11.019		
Mehdi D. Esrafili, Fariba Mohammadian-Sabet			
	NgB.	SD.	23

{{{{{

Comp Quan Chem (CQC)	
species	
▪ (KrOF2)n=2–6 ▪ (XeOF2)n=2–6 clusters	Larger cooperative effects were found in Xe complexes. Comparedto the binary complexes,

	Comp Quan Chem (CQC)	
CQC	Software	Gaussian 09
o Geom opt o Frequency computations	DFT MO6-2X	Theory level
	Small-core energy-consistent relativistic pseudopotential	Xe
	MP2/def2-TZVPPD level	Structure of (ZOF2)n=2,3 clusters
	All-electron def2-TZVPPD triple-f basis set equipped with two sets of polarization and diffusionfunctions	All other atoms
Interaction energy	▪ = Difference of the total energy of the complex and the sum of the isolated monomers in their complex geometry ▪ Corrected using basis set superposition error (BSSE) calculated with CP (counterpoise)method	
MEP analysis	Wave FunctionAnalysis-Surface Analysis Suite (WFA-SAS)	
NBO analysis	NBO 5.0	M06-2X/def2-TZVPPD level of theory
NCI index analysis	MultiWFN program	
Spin-spin coupling constant across the aerogen bond interactions	83Krand 129Xe chemical shielding isotropy values as well as	➔ Gauge included atomic orbital approach ➔ M06-2X/def2-TZVPPD level

}}}}

{{{{{

Aeroogen Bond	NgB.	SD	26

Comp Quan Chem (CQC)	
Single-electron aerogen bond (SEAB)	
LA	LB
▪ KrOF2, KrO3, XeOF2 ; XeO3	Methyl (CH3) radical Ethyl (C2H5) radical

	Comp Quan Chem (CQC)		
CQC	Software		Gaussian 09
Geom opt frequency computations	Theory level	MP2	
	Basis set	aug-cc-pVTZ-PP	Kr; Xe atoms ☞ Includes small-core energy-consistent relativisticpseudopotentials (PP) to account for relativistic effects
		aug-cc-pVTZ	H, C and O atoms
Interaction energy	Corrected by basis set superposition error (BSSE)		

! Topological analysis ! Electron density	o AIM2000 program o MP2/aug-cc-pVTZ(-PP)	
MEP analysis	☞ Wave Function Analysis-Surface Analysis Suite (WFA-SAS)	
NBO analysis	☞ NBO 5.0	o Wave functions generated at HF/aug-cc-pVTZ level

➔ NCI index analysis ➔ Electron localization function (ELF) ➔ Electron density difference (EDD)	✓ MultiWFN program
➔ Spin-spin coupling constant	o Gauge included atomic orbital approach

	✓ M06-2X ✓ All-electron DGDZVP basis set.

Type	Descriptors
MEP	☞ MESP maxima (VS,max, kcal/mol) ☞ MESP minima (VS,min, kcal/mol)
Geometry	☞ Binding distance (Rint, Å) ☞ Binding angles (θO-Z···C, °)
Energy	☞ Interaction energy(Eint, kcal/mol)
Electron Density	☞ Electron Density (Electron Density At BCP) ☞ Laplacian, ∇2ρbcp ☞ Total electron energy density, (HBCP)
Charge	☞ NBO Atomic Charge Change (Δq) Of Z Atom ☞ Charge-Transfer Energy (E(2)) ☞ Net Charge-Transfer (Qct) ☞ Wiberg Bond Index (WBI)
NMR	☞ Absolute Chemical Shielding (Σ, Ppm), 83Kr Or 131Xe ☞ Change with respect to isolated monomer (Δσ, ppm) ☞ Z-C spin-spin constant (J(Z–C), Hz)
Interaction Energies	Ternary complexes ☞ Total Interaction Energies (Eint,Total, Kcal/Mol) ☞ Interaction Energies Of SEAB (Eint, Z···C, Kcal/Mol) ☞ Cooperative energies (Ecoop, kcal/mol)

Single-electron aerogen bonds: Do they exist?	Chemical Physics Letters, 659, 16 August 2016, Pages 196-202 doi.org/10.1016/j.cplett.2016.07.025
Mehdi D. Esrafili, Fariba Mohammadian-Sabet, Mohammad Solimannejad	
	NgB. SD. 26

Exploring "aerogen–hydride" interactions between ZOF2 (Z=Kr, Xe) and metal hydrides: An ab initio study	Chemical Physics Letters, 654, 16 June 2016, Pages 23-28 doi.org/10.1016/j.cplett.2016.05.010
Mehdi D. Esrafili, Fariba Mohammadian-Sabet	
	NgB. SD. 27

{{{{{

Aeroogen Bond	NgB.	SD	28

Comp Quantum Chem (CQC)	
Aerogen bond (NgB)	
LA	LB

▪ XeOF2	o Ethyne, ethene, benzene, pyrrole, o Furan,thiophene
	o Cl^- ; Br^- o Lone pairs o NH3 ; CH3CN

CQC	Software		Gaussian 09
Monomers and complexes ☞ Geom opt ☞ Frequency computations	Theory level	MP2	
	Basis set	aug-cc-pVTZ-PP	Xe atoms ☞ To account for relativistic effects
		aug-cc-pVTZ	H, C and O atoms

Interaction energy	Corrected by basis set superposition error (BSSE)		
Decomposition of Interaction energy	MP2/aug-cc-pVTZ(PP)	! Localized molecular orbital energy decomposition analysis (LMOEDA) method	GAMESS

! Topological analysis ! Electron density	o AIM2000 program o MP2/aug-cc-pVTZ(PP)	
MEP analysis	☞ Wave Function Analysis-Surface Analysis Suite (WFA-SAS) ☞ MP2/aug-cc-pVTZ(PP)	
NBO analysis	☞ NBO 5.0	o Wave functions generated at HF/aug-cc-pVTZ level

➔ NCI index analysis ➔ Electron localization function (ELF) ➔ Electron density difference (EDD)	✓ MultiWFN program

Type	Descriptors
Energy	☞ Second-order perturbation energies (E(2), kcal/mol) ☞ Sum of charge on allatoms of XeOF2 (Q, e) complexes o HF/aug-cc-pVTZ level o
Components of Energy	☞ Electrostatic Energy (ES) ☞ Exchange Energy (EX) ☞ Repulsion Energy (REP) ☞ Polarization Energy (POL) ☞ Dispersion Energy (DISP)

The aerogen–π bonds involving π systems	Chemical Physics Letters, 651, May 2016, Pages 50-55 doi.org/10.1016/j.cplett.2016.03.021
Meng Gao, Jianbo Cheng, Qingzhong Li	
	NgB. SD. 28

}}}}}}

Potential interstellar noble gas molecules: ArOH+ and NeOH+ rovibrational analysis from quantum chemical quartic force fields	Molecular Astrophysics, 2, March 2016, Pages 18-24 doi.org/10.1016/j.molap.2015.12.001
Riley A. Theis, Ryan C. Fortenberry	
	NgB. SD. 29

Comparison of xenon and radon metal halides	Chemical Physics Letters, 638, 1 October 2015, Pages 249-252 doi.org/10.1016/j.cplett.2015.08.064
Christopher C. Lovallo, Mariusz Klobukowski	
	NgB. SD. 30

Main group coordination chemistry at low temperatures: A review of matrix isolated Group 12 to Group 18 complexes	Coordination Chemistry Reviews, 257, Issues 5–6, March 2013, Pages 956-1010 doi.org/10.1016/j.ccr.2012.10.013
Nigel A. Young	
	NgB. SD. 31

Coordination chemistry of the noble gases and noble gas fluorides	Coordination Chemistry Reviews, 257, Issues 5–6, March 2013, Pages 902-909 doi.org/10.1016/j.ccr.2012.07.017
Eric G. Hope	
	NgB. SD. 32

1.10: Studying Highly Reactive Organometallic Complexes with Infrared Spectroscopy: Matrix Isolation, Liquefied Noble Gases, Supercritical Fluids, and Time-resolved IR Spectroscopy	Comprehensive Organometallic Chemistry III, From Fundamentals to Applications Volume 1, 2007, Pages 263-277 doi.org/10.1016/B0-08-045047-4/00011-X
M. W. George, P. Portius	
	NgB. SD. 33

Noble gas compounds and chemistry: a brief review of interrelations and interactions with fluorine-containing species	Journal of Fluorine Chemistry, Volume 121, Issue 1, 1 May 2003, Pages 1-8 doi.org/10.1016/S0022-1139(03)00009-5
Joel F. Liebman, Carol A. Deakyne	
	NgB. SD. 34

Transition metal–noble gas bonding: the next frontier	Chemical Physics Letters, Volume 368, Issues 5–6, 24 January 2003, Pages 589-593 doi.org/10.1016/S0009-2614(02)01913-9
Christopher C Lovallo, Mariusz Klobukowski	
	NgB. SD. 35

Transition metal-noble gas complexes	Advances in Inorganic Chemistry, 52, 2001, Pages 113-150 doi.org/10.1016/S0898-8838(05)52002-6
D. C. Grills, M. W. George	
	NgB. SD. 36

A standard geometrical model for compounds of the main group elements H through I	Journal of Molecular Structure: THEOCHEM, 123, Issues 3–4, August 1985, Pages 399-412 doi.org/10.1016/0166-1280(85)80181-0
Michael R. Peterson, Imre G. Csizmadia	
	NgB. SD. 37

Atom-probe FIM analysis of the interaction of the imaging gas with the surface	Surface Science, 23, Issue 1, October 1970, Pages 112-129 doi.org/10.1016/0039-6028(70)90008-7
E. W. Müller, S. V. Krishnaswamy, S. B. McLane	
	NgB. SD. 38

{{{{

Aeroogen Bond	NgB.	SD	**39**

Comp Quan Chem (CQC)	
Aerogen–pi Interactions	
LA	**LB**
▪ XeO3 ▪ XeF4	o Benzene o Trifluorobenzene, o Hexafluorobenzee

CQC Task	Software		Gaussian 09
Monomers and complexes ☞ Geom opt ☞ Frequency	Theory level	RI-MP2	
	Basis set	aug-cc-pVTZ-PP	Xe atoms ☞ To account for relativistic effects

computations		aug-cc-pVTZ	H, C and O atoms

Type	Computation level	Descriptors
Energies	☞ DF-DFT-SAPT theory ☞ RI-DFT/aug-cc-pVTZ level	☞ SAPT interaction energies (Etotal) → ☞ Electrostatic, ☞ Exchange ☞ Induction ☞ Dispersion

Theoretical Study on the Dual Behavior of XeO3 and XeF4toward Aromatic Rings: Lone Pair–p versus Aerogen–pInteractions	ChemPhysChem, 2015, 16, 3625-3630 DOI : 10.1002/cphc.201500757
Antonio Bauza. and Antonio Frontera	
NgB. SD. 39	

}}}}

Aerogen Bonding Interaction: A New Supramolecular Force?**	Angew. Chem. Int. Ed., 2015, 54, 1- 5 DOI: 10.1002/anie.201502571
Antonio Bauza and Antonio Frontera	
NgB. SD. 40	

Classifying the chemical bonds involving the noble-gas atoms	New J. Chem., 2020,44, 14536-14550 DOI: 10.1039/D0NJ01927E
Stefano Borocci, Felice Grandinetti, Francesca Nunzic and Nico Sanna	
NgB. SD. 41	

Noncovalent Complexes of the Noble-Gas Atoms: Analyzing the Transition from Physical to Chemical Interactions	J. Comput. Chem. 2019, 40, 2318-2328 DOI: 10.1002/jcc.26010
Stefano Borocci, Felice Grandinetti,Nico Sanna, Paola Antoniotti and Francesca Nunzi	
NgB. SD. 42	

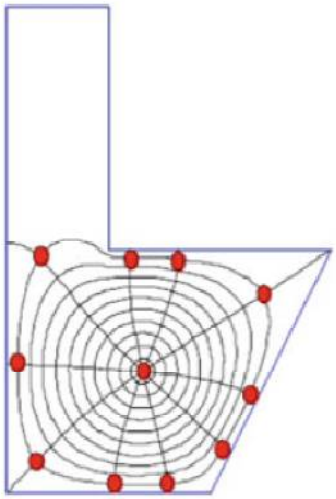
Is Aerogen–p Interaction Capable of Initiating the NoncovalentChemistry of Group 18?	Chem. Asian J. 2015, 10, 2615- 2618 doi.org/10.1002/asia.201500785
Junjian Miao, Bo Song, and Yi Gao	
NgB. SD. 43	

Interaction and Polarization Energy Relationships in σ-Hole and π-Hole Bonding	Crystals 2020, 10, 76 doi.org/10.3390/cryst10020076
Jane S. Murray and Peter Politzer	

What type of bonds? What dynamics? Life!!!

Spiral-like movement inside a huddle of emperor penguins

A huddle of penguins forming L-shaped polygon	Graphical model



Ref	Mahdi Khosravy, Neeraj Gupta, Spiral-like movement inside a huddle of emperor penguins, in Nilesh Patel • Tomonobu Senjyu (Editors), Frontier Applications, of Nature Inspired,Computation, Springer Nature Singapore Pte Ltd. 2020