



فیزیک / فیزیک سامانه های پیچیده و زیستی

شانت

شهبازیان

شماره تماس: ۰۹۹۰۵۰۴۹

رایانامه: sh_shahbazian@sbu.ac.ir

وب سایت:

https://phys.sbu.ac.ir/~sh_shahbazian/home

پروفایل علم سنجی:

http://scimet.sbu.ac.ir/Shant_Shahbazian

تحصیلات

■ کارشناسی ارشد: دانشگاه تهران، شیمی - شیمی فیزیک، ۱۳۷۸ ← ۱۳۸۰

■ دکتری: دانشگاه شهید بهشتی - تهران، شیمی - شیمی فیزیک، ۱۳۸۰ ← ۱۳۸۵

■ کارشناسی: دانشگاه تهران، شیمی گرایش محض، ۱۳۷۴ ← ۱۳۷۸

عالیق پژوهشی

■ مکانیک کوانتومی

■ سیستمهای بس - ذره ای

فعالیت‌های اجرایی

■ معاون پژوهشی دانشکده فیزیک، ۱۳۹۶ ← ۱۳۹۸

■ سرپرست گروه آموزشی شیمی محض، ۱۳۹۴ ← ۱۳۹۵

■ معاون مدیر گروه شیمی محض، ۱۳۹۳ ← ۱۳۹۴

■ استاد راهنما، ۱۳۹۰ ← تا زمان حال

کتب

■ The MC-QTAIM: A framework for extending the “atoms in molecules” analysis beyond purely electronic systems

Shant Shahbazian

Elsevier, Netherlands, 2022, 7-90891-323-0-978

■ Applications of Topological Methods in Molecular Chemistry

Shant Shahbazian

Springer, Switzerland, 2016, 1-29020-319-3-978

■ On the nature of the two-positron bond: evidence for a novel bond type

Mohammad Goli, Dario Bressanini, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.25, pp. 29531-29547, 2023

■ Quantifying errors of electron-proton/muon correlation functionals through the Kohn-Sham inversion of a two-component model system

Nahid Sadat Riyahi, Mohammad Goli, Shant Shahbazian
PHYSICAL REVIEW B, Vol.108, 2023

■ MC-QTAIM analysis reveals an exotic bond in coherently quantum superposed malonaldehyde

Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.25, pp. 5718-5730, 2023

■ Two-component density functional theory for muonic molecules: Inclusion of the electron-positive muon correlation functional

Mohammad Goli, Shant Shahbazian
JOURNAL OF CHEMICAL PHYSICS, Vol.156, 2022

■ The Conceptual and Mathematical Foundations of the MC-QTAIM

Shant Shahbazian
Chemistry, Molecular Sciences and Chemical Engineering, pp. 1-13, 2022

■ On the Nature of the Positronic Bond

Mohammad Goli, Shant Shahbazian
CHEMPHYSCHM, Vol.20, pp. 831-837, 2019

■ Nine questions on energy decomposition analysis

Juan Andrés, Paul W Ayers, Roberto A Boto, Ramon Carbo-Dorca, Henry Chermette, Jerzy Cioslowski, Julia Contreras-Garcia, David L Cooper, Gernot Frenking, Farnaz Heidar-Zadeh, Laurent Joubert, Angel Martin Pendas, Eduard Matito, Istvan Mayer, Alston J Misquitta, Yirong Mo, Julien Pilmé, Paul L A Popelier, Martin Rahm, Eloy Ramos-Cordoba, Pedro Salvador, W. H. Eugen Schwarz, Shant Shahbazian, Bernard Silvi, Miquel Solà, Krzysztof Szalewicz, Vincent Tognetti, Frank Weinhold, Emilie-Laure Zins
JOURNAL OF COMPUTATIONAL CHEMISTRY, Vol.40, pp. 2248-2283, 2019

■ Developing effective electronic-only coupled-cluster and Moller-Plesset perturbation theories for the muonic molecules

Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.20, pp. 16749-16760, 2018

■ Why Bond Critical Points Are Not Bond Critical Points

Shant Shahbazian
CHEMISTRY-A EUROPEAN JOURNAL, Vol.24, pp. 5401-5405, 2018

■ Effective electronic-only KohnSham equations for the muonic molecules

Milad Rayka, Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.20, pp. 8802-8811, 2018

■ Toward a muon-specific electronic structure theory effective electronic HartreeFock equations for muonic molecules

Milad Rayka, Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.20, pp. 4466-4477, 2018

■ Revisiting the foundations of the quantum theory of atoms in molecules Some open problems

Shant Shahbazian
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.118, 2018

■ Incorporating nuclear vibrational energies into the atom in molecules analysis An analytical study

Masumeh Gharabaghi, Shant Shahbazian
JOURNAL OF CHEMICAL PHYSICS, Vol.146, 2017

■ Extending the Domain-Averaged Exchange-Correlation Energies Within the Context of the MC-QTAIM Tracing Subtle Variations Induced by Isotope Substitution
Mohammad Goli, Shant Shahbazian
CHEMPHYSCHM, Vol.17, pp. 3875-3880, 2016

■ Tracing the Fingerprint of Chemical Bonds within the Electron Densities of Hydrocarbons A Comparative Analysis of the Optimized and the Promolecule Densities
Zahra Alimohammadi Keyvani, Shant Shahbazian, Mansoor Zahedi
CHEMPHYSCHM, Vol.17, pp. 3260-3268, 2016

■ To What Extent are Atoms in Molecules Structures of Hydrocarbons Reproducible from the Promolecule Electron Densities
Zahra Alimohammadi Keyvani, Shant Shahbazian, Mansoor Zahedi
CHEMISTRY-A EUROPEAN JOURNAL, Vol.22, pp. 5003-5009, 2016

■ Muon-Substituted Malonaldehyde Transforming a Transition State into a Stable Structure by Isotope Substitution
Mohammad Goli, Shant Shahbazian
CHEMISTRY-A EUROPEAN JOURNAL, Vol.22, pp. 2525-2531, 2016

■ Seeking Extremes in Molecular Design To What Extent May Two Non-Bonded Hydrogen Atoms be Squeezed in a Hydrocarbon
Rohoullah Firouzi, Shant Shahbazian
CHEMPHYSCHM, Vol.17, pp. 51-54, 2016

■ Some implications of the Hartree product treatment of the quantum nuclei in the ab initio nuclear electronic orbital methodology
Masumeh Gharabaghi, Shant Shahbazian
PHYSICS LETTERS A, Vol.380, pp. 3983-3987, 2016

■ Topological and AIM analyses beyond the Born Oppenheimer paradigm New opportunities
Mohammad Goli, Shant Shahbazian
Computational and Theoretical Chemistry, Vol.1053, pp. 96-105, 2015

■ Where to place the positive muon in the Periodic Table
Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.17, pp. 7023-7037, 2015

■ Six questions on topology in theoretical chemistry
Ayers Paul , Boyd Russell, Bultinck Patrick, Caffarel Michel, Carb?-Dorca Ramon, Caus? Mauro, Cioslowski Jerzy, Contreras-Garcia Julia, Cooper David, Coppens Philip, Gatti Carlo, Grabowsky Simon, Lazzaretti Paolo, Macchi Piero, Mart?n Pend?s angel, Popelier Paul, Ruedenberg Klaus, Rzepa Henry, Savin Andreas, Sax Alexander, Schwarz Eugen, Shant Shahbazian, Silvi Bernard, Solà Miquel, Tsirelson Vladimir
Computational and Theoretical Chemistry, Vol.1053, pp. 2-16, 2015

■ What does shape a topological atom
Hamidreza Jouypazadeh, Shant Shahbazian
Foundations of Chemistry, Vol.16, pp. 63-75, 2014

■ Letter to the editor Are there really atoms in molecules
Shant Shahbazian
Foundations of Chemistry, Vol.16, pp. 77-84, 2014

■ Deciphering the chemical nature of the exotic isotopes of hydrogen by the MC-QTAIM analysis the positively charged muon and the muonic helium as new members of the periodic table
Mohammad Goli, Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.16, pp. 6602-6613, 2014

■ Toward a Consistent Interpretation of the QTAIM Tortuous Link between Chemical Bonds Interactions and Bond/Line Paths
, Shant Shahbazian,
CHEMISTRY-A EUROPEAN JOURNAL, Vol.20, pp. 10140-10152, 2014

■ Hidden aspects of the Structural theory of chemistry MC-QTAIM analysis reveals alchemical transformation from

a triatomic to a diatomic structure

Mohammad Goli, Shant Shahbazian

PHYSICAL CHEMISTRY

 CHEMICAL PHYSICS, Vol.17, pp. 245-255, 2014

- Seeking for ultrashort non-bonded hydrogen hydrogen contacts in some rigid hydrocarbons and their chlorinated derivatives

, Shant Shahbazian

STRUCTURAL CHEMISTRY, pp. 1297-1304, 2014

- Toward the multi-component of quantum theory of atoms in molecules a variational derivation

Mohammad Goli, Shant Shahbazian

THEORETICAL CHEMISTRY ACCOUNTS, Vol.132, pp. 1-17, 2013

- Beyond the orthodox QTAIM motivations current status prospects and challenges

Shant Shahbazian

Foundations of Chemistry, Vol.15, pp. 287-302, 2013

- The two-component quantum theory of atoms in molecules (TC-QTAIM) tesnor formulation and its implications

Mohammad Goli, Shant Shahbazian

THEORETICAL CHEMISTRY ACCOUNTS, Vol.132, pp. 1-14, 2013

- The two-component quantum theory of atoms in molecules (TC-QTAIM) the unified theory of localization/delocalization of electrons nuclei and exotic elementary particles

Mohammad Goli, Shant Shahbazian

THEORETICAL CHEMISTRY ACCOUNTS, Vol.132, pp. 1-22, 2013

- Comment on Austere quantum mechanics as a reductive basis for chemistry

Shant Shahbazian

Foundations of Chemistry, Vol.15, pp. 327-334, 2013

- The Two-Component Quantum Theory of Atoms in Molecules (TC-QTAIM) Foundations

Mohammad Goli, Shant Shahbazian

THEORETICAL CHEMISTRY ACCOUNTS, Vol.131, pp. 1-19, 2012

- Toward a Regional Quantum Description of the Positronic Systems Primary Considerations

payam nasertayoob, Mohammad Goli, Shant Shahbazian

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.111, pp. 1970-1981, 2011

- Toward a fuzzy atom view within the context of the quantum theory of atoms in molecules quasi-atoms

Farnaz Heydarzadeh, Shant Shahbazian

THEORETICAL CHEMISTRY ACCOUNTS, Vol.128, pp. 175-181, 2011

- The Laplacian of Electron Density versus NICSzz Scan Measuring Magnetic Aromaticity among Molecules with Different Atom Types

Cina Foroutan-Nejad, Zahra Badri, Shant Shahbazian, Parviz Rashidi-Ranjbar

JOURNAL OF PHYSICAL CHEMISTRY A, Vol.115, pp. 12708-12714, 2011

- The Quantum Divided Basins A New Class of Quantum Subsystems

Farnaz Heydarzadeh, Shant Shahbazian

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.111, pp. 2788-2801, 2011

- The Quantum Theory of Atoms in Positronic Molecules The Subsystem Variational Procedure

Farnaz Heydarzadeh, Shant Shahbazian

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.111, pp. 1999-2013, 2011

- Reply to the Comment on The electron density vs. NICS scan a new approach to assess aromaticity in molecules with different ring sizes by A. Stanger Phys. Chem. Chem. Phys. 2011 13 DOI 10.1039/c0cp02407d

Parviz Rashidi-Ranjbar, , Shant Shahbazian

PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.13, pp. 12655-12658, 2011

- Letter to the Editor The Mathematical Soundness and the Physical Content of the Subsystem Variational Procedure of the QTAIM

■ A Dissected Ring Current Model for Assessing Magnetic Aromaticity A General Approach for both Organic and Inorganic Rings

, Shant Shahbazian,,
JOURNAL OF COMPUTATIONAL CHEMISTRY, Vol.32, pp. 2422-2431, 2011

■ The critical re-evaluation of the aromatic/antiaromatic nature of Ti3(CO)3 a missed opportunity

, Shant Shahbazian,
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.21, pp. 4576-4582, 2011

■ The Quantum Theory of Atoms in Positronic Molecules A case study on diatomic species

Mohammad Goli, Shant Shahbazian
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.111, pp. 1982-1998, 2011

■ Atoms in molecules beyond Born Oppenheimer paradigm

Mohammad Goli, Shant Shahbazian
THEORETICAL CHEMISTRY ACCOUNTS, Vol.129, pp. 235-245, 2011

■ Revisiting the foundations of the quantum theory of atoms in molecules The subsystem variational procedure and the finite nuclear models

, Shant Shahbazian
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.110, pp. 1188-1196, 2010

■ The Electron Density vs. NICS Scan A New Approach to Assess Aromaticity in Molecules with Different Ring Sizes

Shant Shahbazian
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.12, pp. 12630-12637, 2010

■ The topological analysis of electronic charge densities A reassessment of foundations

Shant Shahbazian,
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.869, pp. 53-58, 2008

■ A Simple and Convenient Strategy for the Synthesis of Tolanophanes Synthesis Characterization and Conformational Analysis of a Novel Tolanophane

Khosro Jadidi, Shant Shahbazian
SUPRAMOLECULAR CHEMISTRY, Vol.20, pp. 327-333, 2008

■ Atomic basins with more than a single nucleus a theochem fact or a mathematical artifact

Shant Shahbazian,
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.894, pp. 20-22, 2008

■ Revisiting the Foundations of the Quantum Theory of Atoms in Molecules Toward a Rigorous Definition of Topological Atoms

Shant Shahbazian,
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.109, pp. 726-732, 2008

■ Revisiting the Foundations of Quantum Theory of Atoms in Molecules (QTAIM) The Variational Procedure and the Zero-Flux Conditions

Shant Shahbazian,
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.108, pp. 1477-1484, 2008

■ A Computational Study on Some Viable Targets for Gas-Phase Synthesis of Metal Complexes of the Cyclic (B6C)-2 and Their Bonding Pattern

Shant Shahbazian, Shadi Alimohammadi Choshli
JOURNAL OF PHYSICAL CHEMISTRY A, Vol.112, pp. 10365-10377, 2008

■ An ab initio study of geometry and vibrational spectrum of cyclic (B6C)(-2) The out-of-plane bending problem

Shant Shahbazian
CHEMICAL PHYSICS LETTERS, Vol.443, pp. 147-151, 2007

■ Ab initio Post-HF study of electronic charge density distribution of cyclic (B6C)-2 Concrete evidence of a novel bonding pattern

Shant Shahbazian,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.822, pp. 116-121, 2007

■ کوانتمو و انرژی

شانت شهبازیان

دانشنامه انرژی، نسخه ۱، صفحات: ۱-۳، ۱۳۹۴

■ انرژی تاریک

شانت شهبازیان

دانشنامه انرژی، نسخه ۱، صفحات: ۱-۱، ۱۳۹۴

■ قانون پایستگی انرژی

شانت شهبازیان

دانشنامه انرژی، نسخه ۱، صفحات: ۱-۲، ۱۳۹۴

■ انرژی نقطه صفر

شانت شهبازیان

دانشنامه انرژی، نسخه ۱، صفحات: ۳-۵، ۱۳۹۴

مقالات علمی ارائه شده در همایش‌ها

■ Extending chemical concepts beyond chemistry: Revealing "Atoms in molecules" and chemical bonds in the positronic and muonic molecules

Shant Shahbazian, Mohammad Goli

IUPAC CCCE 2021 Virtual (Chemistry at the frontiers), pp.584-584

■ The Multi-Component Quantum Theory of Atoms in Molecules (MC-QTAIM) New developments and novel opportunities

Shant Shahbazian

8th conference of modern methods in quantum chemistry

■ the two-component Quantum theory of Atoms in molecules

Shant Shahbazian

TCC012-I, pp.89-90

■ Why bond critical points are not bond critical points

شانت شهبازیان

Seventh Theoretical and Computational Chemistry Workshop، ۱-۱، صفحات:

Effective electronic structure theory for partially non-Born-Oppenheimer systems ■

شانت شهبازیان

ششمین کارگاه و سمینار شیمی نظری و محاسباتی، صفحات: ۶-۶

■ استفاده از اتم میونیوم برای بررسی پیوند کربن-کربن مرکزی معکوس شده در ۱،۱،۱ پروپلان

محمد گلی، شانت شهبازیان

بیست و سومین کنفرانس بهاره فیزیک، صفحات: ۱-۳

■ توسعه مدل هارمونیوم غریب به منظور بررسی همبستگی الکترون - ذره باردار مشتث در سامانه های کواتتومی دو جزی

ناهید سادات ریاحی

۱۳۹۰۲

■ بررسی تحلیلی خواص هسته ها در چارچوب نظریه اتم ها در مولکول های چند جزئی
معصومه قراباغی

۱۳۹۶

■ بررسی امکان باز تولید ویژگی های مولکولی بر اساس خصوصیات اتم های آزاد: چگالی الکترونی و انرژی همبستگی
زهرا علی محمدی کیوانی

۱۳۹۵

■ توسعه و کاربردهای نظریه کواتتومی اتم ها در مولکول های چند جزئی
محمد گلی

۱۳۹۴

پایان نامه های کارشناسی ارشد

■ توسعه نظریه ساختار الکترونی موثر برای سیستم های مولکولی میونی معادلات هارتی - فاک و معادلات کوهن - شام
میلاد رایکا

۱۳۹۶

■ استفاده از نظریه فاجعه بنیادی در تحلیل توپولوژیک چگالی الکترونی
زهرا خداداد

۱۳۹۵

■ بررسی مدل خوش ذرات آلفای هسته ای با استفاده از تحلیل توپولوژیک چگالی نوکلئونی
حديثه شيرزادی

۱۳۹۴

مدل سازی جریان های الکترونی القائی ناشی از میدان مغناطیسی خارجی با استفاده از قوانین الکترومغناطیس کلاسیک در برخی هیدروکربن
■ . های آروماتیک مسطح

الهام حرم زاده کلیائی

۱۳۹۲

■ بررسی محاسباتی ساختار ظرفی چگالی الکترونی اتم ها و بازه های کواتتومی تقسیم شده ای هسته ای
علیرضا معرفت خواه

۱۳۹۱

■ بررسی سطوح انرژی پتانسیل غیر آدیاباتیک و چگالی های الکترونی در چارچوب مدل کواتتومی هوک - کالوگرو
حمیدرضا جوپیاز اده

۱۳۹۰

