

مشخصات فردی

نام خانوادگی : اسرافیلی دیزجی
شروع به خدمت :
گروه آموزشی : شیمی
فاکس :
رشته تحصیلی: شیمی کوانتوم
تاریخ ایجاد : دهم شهریور ۱۳۹۳

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تاریخ تولد : ۱۳۶۰

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محل تحصیل : دانشگاه تربیت مدرس تهران

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بیوگرافی

توضیحات

خوش آمدید

صفحه شخصی

- نام : مهدی
- نام خانوادگی: اسرافیلی دیزجی
- محل تولد: آذربایجان شرقی، شهرستان شبستر
- تاریخ تولد: 1/6/1360
- وضعیت تاهل: متاهل دارای دو فرزند

سوابق تحصیلی

سوابق تحصیلی

سال اخذ مدرک	شهر محل تحصیل	کشور محل تحصیل	دانشگاه محل تحصیل	مدرک تحصیلی	گرایش	رشته تحصیلی
1389	کیوتو	ژاپن	کیوتو	visiting scholar	شیمی کوانتم	شیمی
1389	تهران	ایران	تربیت مدرس	دکتری	شیمی کوانتم	شیمی
1385	تهران	ایران	تربیت مدرس	کارشناسی ارشد	شیمی فیزیک	شیمی
1383	تهران	ایران	تربیت معلم تهران (خوارزمی)	کارشناسی	محض	شیمی

اختراعات

کارگاه ها

علایق

طرح درس

زمینه های پژوهشی

زمینه های تحقیقاتی مورد علاقه:

- برهمکنشهای بین مولکولی
- نانو شیمی
- شیمی سطح
- بررسی نظری واکنشهای شیمیایی کاتالیز شده توسط نانوکاتالیستها
- Configuration Interaction
- Symmetry Adapted Perturbation Theory
- مطالعه خواص مولکولی با استفاده از شبیه سازی دینامیک مولکولی (MD)
- مطالعه اثرات نسبیتی در شیمی فلزات سنگین

همکاری با تحریریه مجلات علمی

پروژه های تحقیقاتی خارج از دانشگاه

پروژه های تحقیقاتی

1. دکتر صادق افشاری (سال 94)
2. دکتر مرتضی روحانی (سال 94)

کارشناسی ارشد:

1. وحیده عزیزاده (بررسی ساختار الکترونی کمپلکسهای لانتانیدی شامل لیگاندهای فسفیدی و کربونیلی به کمک روشهای محاسباتی)
2. هاشم احمدین (بررسی نظری اثر پیوندهای هیدروژنی درون و برون مولکولی بر روی تانسورهای پوشیدگی شیمیایی و شیب میدان الکتریکی اتمهای اکسیژن، هیدروژن و کربن در ساختار بلوری فرمهای α و β سلولز)
3. مجتبی بیژنی (بررسی نظری جذب برخی گازها بر روی نانوتیوبهای کربنی و فولرنها: کاربرد یونهای فلزی نظیر Li^+ ، Na^+ و Mg^{2+} برای بهبود جذب H_2 و O_2)
4. سکینه محمدزاده (بررسی ساختار الکترونی و مولکولی نانولوله های سلولیکون-کاربیدبا استفاده از نظریه تابعیت چگالی)
5. فیروزه زرین فر (مطالعه نظری ساختار الکترونی نانو تیوبهای بورنیترویدی و بورفسفری: بررسی اثرات ساختاری و ناخالصی های کربن بر روی پارامترهای تشدید مغناطیس هسته)
6. مهشاد وکیلی گرمودی (بررسی نظری قدرت و ماهیت برهمکنشهای غیر کووالانسی هالوژن-هالوژن، هالوژن-نیتروژن و هالوژن-فسفر به کمک روشهای شیمی کوانتمی)
7. پروین فاتحی قلعه (بررسی اثرات هم افزایی در پیوندهای هالوژنی و لیتیومی)
8. پریسا جویبان (مطالعه نظری کمپلکسهای گازهای نجیب به کمک روشهای مکانیک کوانتمی)
9. رقیه نور آذر (بررسی واکنش پذیری سطح نانولوله های غیر کربنی و سینتیک جذب سطحی برخی مولکولها به کمک محاسبات شیمی کوانتمی)
10. اکرم سید اسماعیلی (بررسی نظری اثرات ناخالصیهای لانتانیدی و اکتینیدی در نانولوله های BC3 و BC2N)
11. نصیبه سعیدی (بررسی نظری فعالسازی مولکول اکسیژن بر روس سطوح گرافنی و نانولوله های داپ شده با اتمهای غیر فلزی)
12. نفیسه محبی راد (بررسی نظری جذب و تفکیک مولکولهای آلی نظیر الکها و آمیدها بر روی فولرنها)
13. وحیده معصومی (بررسی واکنش تجزیه ترکیب هیدروژن دار نظیر هیدرازین و مشتقات مربوطه بر روی نانو ساختار به کمک روشهای مکانیک کوانتمی)
14. فریبا محمدیان-ثابت (بررسی نظری اثرات ناخالصیهای غیر فلزی نظیر سیلیسم و آلومنیوم بر روی سینتیک واکنشهای هیدروژن زدایی کاتالیز شده بوسیله نانولوله های کربنی-غیر کربنی و ماهیت برهمکنشهای بین مولکولی σ -hole و π -hole در فاز گازی)
15. پریسا نعمت الهی (بررسی نظری مکانیزم واکنشهای اکسایش-کاهش بر روی نانو ساختارهای کربنی و غیر کربنی)
16. فهیمه شریفی (مکانیزم واکنش اکسیداسیون منوکسید کربن بر روی گرافن و گرافن اکسید به کمک روشهای شیمی کوانتمی)
17. هادی عبدالله پور (بررسی اثر میدان الکتریکی بر روی سینتیک اکسیداسیون گاز مونوکسید کربن بر روی گرافن و گرافن دوبه شده با فلزات)
18. سهیلا اسدالهی (بررسی قدرت و ماهیت برهمکنشهای غیر کووالانسی σ -hole و π -hole به کمک محاسبات مکانیک کوانتمی)
19. صفا حیدری (بررسی نظری حذف آلاینده های گازی نظیر NO ، N_2O و CO به کمک گرافن داپ شده با اتمهای فلزی)
20. پریسالادات موسویان (بررسی نظری قدرت و ماهیت برهمکنش های دهنده-گیرنده در عناصر گروههای VIII-III به کمک محاسبات ab initio سطح بالا)

عضویت در کمیته ها و شوراهای

- 1- عضو شورای دانشگاه از سال 1395 (ادامه دار)
- 2- عضو شورای پژوهشی دانشگاه از سال 1392 (ادامه دار)
- 3- عضو کمیته نانو فناوری از سال 1391 (ادامه دار)
- 4- عضو کارگروه بررسی تواناییهای علمی گروه شیمی از سال 1392 (ادامه دار)

عضویت در مجامع علمی و انجمن ها

عضویت در انجمن ها و مجامع علمی

سال پایان	سال شروع	نوع همکاری و سمت	محل فعالیت مجمع	نام انجمن یا مجمع
	1386		تهران	انجمن شیمی ایران

تشویق ها

افتخارات آموزشی:

- فارغ التحصیل رتبه اول مقطع کارشناسی ارشد رشته شیمی فیزیک سال 1385
- کسب رتبه دوم امتحان ورودی دکتری در سال 1385
- نفر اول آزمون جامع رشته شیمی فیزیک سال 1387
- عضو دفتر استعدادهای درخشان دانشگاه تربیت مدرس 1387
- عضو بنیاد ملی نخبگان 1387
- نفر برگزیده به عنوان نخبه برتر در دومین همایش نخبگان و دریافت لوح تقدیر از معاون فناوری رئیس جمهور در سال 1387
- فارغ التحصیل رتبه اول مقطع دکتری رشته شیمی فیزیک سال 1389
- استاد نمونه دانشکده علوم پایه سال 1396

افتخارات پژوهشی:

- پژوهشگر برتر دانشکده علوم پایه دانشگاه مراغه در سال 1391
- دریافت گرنت پژوهشی ویژه استادیاران جوان از بنیاد ملی نخبگان (1392)
- پژوهشگر برتر دانشگاه مراغه در سال 1392
- پژوهشگر برتر استان آذربایجان شرقی در سال 1393
- انتخاب شده به عنوان (جز 100 نفر) محقق برتر در جشنواره تجلیل از برترینهای نانو کشور در 1393
- انتخاب شده به عنوان (جز 100 نفر) محقق برتر در جشنواره تجلیل از برترینهای نانو کشور در 1395

سابقه ارائه خدمات آموزشی

(سال)ادامه دار	عنوان درس	مقطع تحصیلی	موسسه محل تدریس
1391	شیمی نظری ساختارهای نانو	کارشناسی ارشد	دانشگاه مراغه
1391	شیمی کوانتوم 2	کارشناسی ارشد	دانشگاه مراغه
1391	ترمودینامیک آماری	کارشناسی ارشد	دانشگاه مراغه
1387	شیمی فیزیک 1	کارشناسی	دانشگاه مراغه
1388	شیمی فیزیک 2	کارشناسی	دانشگاه مراغه
1389	مبانی شیمی کوانتم	کارشناسی	دانشگاه مراغه
1389	شیمی عمومی	کارشناسی	دانشگاه مراغه
1390	زبان تخصصی شیمی	کارشناسی	دانشگاه مراغه
1389	شیمی فیزیک پیشرفته	کارشناسی ارشد	دانشگاه مراغه

The enhancing effect of a cation- π interaction on the cooperativity of halogen bonds: A computational study

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The strengthening effect of a hydrogen or lithium bond on the $\text{Z}\cdots\text{N}$ aerogen bond (Z= Ar, Kr and Xe): a comparative study

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Symmetric bifurcated halogen bonds: Substituent and cooperative effects

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Cooperativity in bifurcated lithium-bonded complexes: A DFT study

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International Symposium on Molecular Theory for Real Systems, Kyoto University, Kyoto, 2010 (Poster)

A DFT investigation on atomic oxygen, O₂ and O₃ adsorption on (5,0) SWCNT

2th Nanotechnology Seminar, University of Razi, Kermanshah, 2008 (Oral)

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Investigation of substitution effects in lanthanides M(X₂C=O)₂ complexes (M=La-Lu, X=H, F, Cl, Br, CN, OH, and CH₃)

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On the nature of Mg-L interactions (L= BF, CO, N₂, NH₃ and H₂O): A symmetric-adapted perturbation theory (SAPT) study

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

A QTAIM study on carbon-doping at different sites of (8,0) BNNTs

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

A comparative study of carbon, boron-nitride and silicon-carbide nanotubes based on surface electrostatic potential and QTAIM analysis

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

A DFT study of hydrogen adsorption on Ln@B₁₆N₁₆ fullerene-like nanocluster (Ln: La, Gd and Ln)

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

A theoretical study on bonding and energy aspects of [Ln(DOTA)]⁻ and [Ln(DOTA).H₂O]⁻ complexes (Ln=Eu³⁺, Ho³⁺)

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

A DFT investigation on NMR spin-spin coupling constants in Ibuprofen drugs

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

Theoretical Study of Cooperative effects in α-glycylglycine clusters

15th Iranian Physical Chemistry Seminar, University of Tehran, 2012 (Poster)

Interaction of B₁₂N₁₂ with HCl: Ab initio-, QTAIM-, and NBO-Based study

Nano Conference, Sharif University, Tehran, Iran, 2013 (Poster)

A Theoretical Study on the Possibility of Using Boron Nitride Nanotubes as Metal-Free Catalysts for Methanol Dehydrogenation

17th Iranian Physical Chemistry Seminar, Khajeh Nasir University, 2014 (Poster)

Competition and Interplay between the Lithium Bonding and Hydrogen Bonding: R₃C...HY...LiY and R₃C...LiY...HY Triads (R=H, CH₃; Y=CN, NC) as a Working Model

برنامه درسی ترم جاری

17th Iranian Physical Chemistry Seminar, Khajeh Nasir University, 2014 (Poster)

Interplay and Competition between the Lithium Bonding and Halogen Bonding: R₃C...XCN...LiCN and R₃C...LiCN...XCN (R=H, CH₃; X=Cl, Br) as a Working Model

سایر

17th Iranian Physical Chemistry Seminar, Khajeh Nasir University, 2014 (Poster)

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Mutual Influence between S...N(C) and Hydrogen/Lithium/Halogen Bonds: Competition and Interplay between π-Hole and σ-Hole Interactions

17th Iranian Physical Chemistry Seminar, Khajeh Nasir University, 2014 (Poster)

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- تسلط به زبان ترکی (آذربایجانی و استامبولی)
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Halogen Bond Interactions Enhanced by Sodium Bonds: A Theoretical Evidence for Cooperative Effects in NCX...NCNa...NCY Complexes (X = F, Cl, Br; Y = H, F, OH)

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