【个人信息】

姓名：刘晓洁　　职称：教授、博士生导师
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【个人情况综述】

刘晓洁，理学博士，教授。主要从事低维新颖纳米材料的生长机制、性质及其应用的理论研究；利用量子尺寸效应设计表面化学反应活性可控的金属纳米材料；准原子基最小轨道的微观成键机理研究；半导体改性、氢键等弱相互作用体系、新颖纳米材料的结构搜索研究等。在主流学术期刊(如 Phys. Rev. B、J. Phys. Chem. C、Adv. Mater.、Phys. Rev. Lett.等)上发表 SCI 论文 30 余篇，其中受邀发表综述论文 2 篇，Google 引用>900 余次(4 篇文章引用>100 次)，先后主持和参与国家自然科学基金 7 余项。

【学习工作简历】

2014.05-至今　东北师范大学物理学院/量子科学中心，副教授、教授。
2012.02-2014.04　北京计算科学研究中心，博士后。
2009.09-2011.04　美国能源部 Ames 实验室，Iowa State University, 访问学者。
2006.08-2011.12　吉林大学理论化学研究所量子化学专业，获理学博士学位。
2002.08-2006.07　辽宁师范大学化学化工学院应用化学专业，获理学学士学位。

【教学工作】

本　科：《固体物理》、《计算物理基础》、《物理前沿问题专题》、《探索物理实验》
研究生：《计算物理》

【主要科研方向】

1．新颖纳米材料的生长与性质研究；
2．半导体材料物化性质改性；
3．材料设计与结构搜索；

【主要科研项目】

1. 国家自然科学基金-平台项目：东北师范大学材料计算与模拟研究团队及其学术交流平台，40 万，2018.01-2018.12，项目负责人
2. 国家自然科学基金-面上项目：金属插入对石墨烯物化性质调控的理论研究，62 万，2016.01-2019.12，项目负责人
3. 东北师范大学紫外光发射材料与技术教育部重点实验室开放课题项目：氧缺陷对二氧化钛光学性质影响的理论研究，5 万，2016.01-2016.12，项目负责人
4. 吉林省科技厅-青年科研基金：石墨烯表面金属纳米材料物化性质及其应用的研究，6 万，2015.01-2017.12，项目负责人
5. 国家自然科学基金-青年基金：石墨烯表面金属纳米材料生长形貌以及生长机制的探索，25 万，2013.01-2015.12，项目负责人
6. 中国博士后科学基金第六批特别资助：石墨烯表面金属纳米材料生长的理论研究，15 万，2013.06-2014.08，项目负责人

【主要科研成果】

学术论文：

1. **X. Liu**, C.Z. Wang, M. Hupalo, Y.X. Yao, M.C. Tringides, W.C. Lu, K.M. Ho, *Adsorption and*

growth morphology of rare-earth metals on graphene studied by ab initio calculations and scanning tunneling microscopy, Phys. Rev. B 82, 245408 (2010).

2. M. Hupalo, **X. Liu**, C.Z. Wang, W.C. Lu, Y.X. Yao, K.M. Ho and M.C. Tringides, *Metal Nanostructure Formation on Graphene: Weak versus Strong Bonding*, Adv. Mater. 23, 2082 (2011).

3. **X. Liu**, C.Z. Wang, Y.X. Yao, W.C. Lu, M. Hupalo, M.C. Tringides and K.M. Ho, *Bonding and charge transfer by metal adatom adsorption on graphene*, Phys. Rev. B 83, 235411 (2011).

4. **X. Liu**, W.C. Lu, C.Z. Wang, K.M. Ho, *Energetic and fragmentation stability of water clusters* $(H_2O)_n$*, n=2-30*, Chem. Phys. Lett. 508, 270 (2011).

5. **X. Liu**, C.Z. Wang, M. Hupalo, W.C. Lu, P.A. Thiel, K.M. Ho, and M.C. Tringides, *Fe-Fe adatom interaction and growth morphology on graphene*, Phys. Rev. B 84, 235446 (2011).

6. **X. Liu**, C.Z. Wang, M. Hupalo, W.C. Lu, M.C. Tringides, Y.X. Yao and K.M. Ho, *Metals on graphene: correlation between adatom adsorption behavior and growth morphology*, Phys. Chem. Chem. Phys. 14, 9157 (2012).

7. S.M. Binz, M. Hupalo, **X. Liu**, C.Z. Wang, W.C. Lu, P.A. Thiel, K.M. Ho, E.H. Conrad and M.C. Tringides, *High Island Densities and Long Range Repulsive Interactions: Fe on Epitaxial Graphene*, Phys. Rev. Lett. 109, 026103 (2012).

8. A.K. Engstfeld, H.E. Hoster, R.J. Behm, L.D. Roelofs, **X. Liu**, C.Z. Wang, Y. Han and J.W. Evans, *Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling*, Phys. Rev. B 86, 085442 (2012).

9. **X. Liu**, M. Hupalo, C.Z. Wang, W.C. Lu, P.A. Thiel, K.M. Ho and M.C. Tringides, *Growth morphology and thermal stability of metal islands on graphene*, Phys. Rev. B 86, 081414(R) (2012).

10. D. Shao, **X. Liu**, N. Lu, C.Z. Wang, K.M. Ho, M.C. Tringides and P.A. Thiel, *Effects of Oxygen on the Stability of Ag islands on Si(111)-7x7*, Surf. Sci. 606, 1871 (2012).

11. **X. Liu**, C.Z. Wang, M. Hupalo, H.-Q. Lin, K.M. Ho and M.C. Tringides, *Metal on graphene: Interaction, Growth Morphology, and Thermal Stability*, Crystals, Invited review paper, 3, 79-111 (3013).

12. G.P. Zhang, **X. Liu***, C.Z. Wang, Y.X. Yao, J. Zhang and K.M. Ho, *Electronic and transport properties of graphene nanoribbon mediated by metal adatom: A study by QUAMBO-NEGF approach*, J. Phys.: Condens. Matter, 25, 105302 (2013).

13. **X. Liu**, C.-Z. Wang, M. Hupalo, H.-Q. Lin, K.-M. Ho and M. C. Tringides, *Quantum confinement induced oscillatory electric field on stepped Pb(111) film and its influence on surface reactivity*, Phys. Rev. B 89, 041401(R) 2014.

14. **X. Liu**, C.-Z. Wang, H.-Q. Lin and K.-M. Ho, *Magnetic moment enhancement for* Mn_7 *cluster on graphene*, J Phys. Chem. C 118, 19123-19128 (2014).

15. **X. Liu**, C.-Z. Wang, M. Hupalo, H.-Q. Lin, K.-M. Ho and M. C. Tringides, *Structures and magnetic properties of Fe clusters on graphene*, Phys. Rev. B 90, 155444 (2014).

16. **X. Liu**, C.-Z. Wang, H.-Q. Lin and K.-M. Ho, *Charge oscillation and interaction between potassium adatoms on graphene by first-principles calculations*, Phys. Rev. B 91, 035415 (2015).

17. **X. Liu**, J. W. Evans, M. C. Tringides, Y. Han, M. Hupalo, H.-Q. Lin, K.-M. Ho, D. Appy, P. A. Thiel and C.-Z. Wang, *Growth Morphology and Properties of Metals on Graphene*, Progress in Surface Science, Invited review paper, 90, 397-443 (2015).

18. **X. Liu** and C.-Z. Wang, *Growth mode and structures of magnetic Mn clusters on graphene*,

RSC Adv., 6, 64595 (2016).
19. **X. Liu**, C.-Z. Wang, M. Hupalo, H.-Q. Lin, K.-M. Ho, P. A. Thiel and M. C. Tringides, *Metal intercalation-induced selective adatom mass transport on graphene*, Nano Research, 9, 1434–1441 (2016).
20. **X. Liu**, C.-Z. Wang, M. Hupalo, K.-M. Ho, P. A. Thiel and M. C. Tringides, *Interplay between surface and surface resonance states on height selective stability of fcc Dy(111) film at nanoscale*, Phys. Chem. Chem. Phys., 18, 31238 (2016).
21. **X. Liu** and C.-Z. Wang, I*nterplay between quantum confinement and surface effects in thickness selective stability of thin Ag and Eu films*, J. Phys.: Condens. Matter 29, 185504 (2017).
22. **X. Liu** and C.-Z. Wang, *Transition metal partially supported graphene: Magnetism and oscillatory electrostatic potentials*, J. Appl. Phys., 122, 055303 (2017).
23. C. Du, L. Yu, **X. Liu***, L. Liu and C.-Z. Wang, *Oscillatory electrostatic potential on graphene induced by group IV element decoration*, Sci. Rep., 7, 13152 (2017).
24. L. Yu, C. Du and **X. Liu***, *Dy adsorption and penetration on defected graphene by first principles calculations*, Mater. Res. Express 5, 025022 (2018).
25. C. Du, Y. Yang, **X. Liu*** and G. Shan, *First-principles study of electronic properties of Cu doped Ag_2S*, J. Phys.: Condens. Matter 30, 425502 (2018).
26. Y. Liu, H. Ji, **X. Liu*** and W. C. Lu, *Ring-Stacking Water Clusters: Morphology and Stabilities*, ChemistryOpen 8, 210–218 (2019).
27. L. Li, K. Jin, C. Du and **X. Liu***, *The effect of oxidation on the electronic properties of penta-graphene: first-principles calculation*, RSC Adv., 9, 8253 (2019).
28. W. Yan and **X. Liu***, Niobium-Doped TiO_2: Effect of an Interstitial Oxygen Atom on the Charge State of Niobium, Inorg. Chem., 58, 3090−3098 (2019).
29. W. Yan, X. Yuan and **X. Liu***, *Theoretical investigation of dissociative and non-dissociative acetic-acid on TiO_2-B surfaces*, Appl. Surf. Sci., 494, 850-858 (2019).
30. C. Du, K. Jin and **X. Liu***, *Electronic and optical properties of gold-doped endohedral fullerenes*, J. Mater. Sci., 55, 12980-12994 (2020).
31. Y. Zhao, M. Song, X. Yang, J. Yang, C. Du, G. Wang, J. Yi, G. Shan*, D. Li*, L Liu*, D. Yan, Y. Li, **X. Liu***, *Amorphous $Ag_{2-x}Cu_xS$ quantum dots: "all-in-one" theranostic nanomedicines for near-infrared flfluorescence/photoacoustics dual-modal imaging-guided photothermal therapy*, Chem. Eng. J., 399, 125777 (2020).
32. J. Sun, Z. Xu and **X. Liu***, *Structures and stabilities of glycine and water complexes*, Chem. Phys., 528, 110528 (2020).
33. C. Du, J. Tian and **X. Liu***, *Effect of intrinsic vacancy defects on the electronic properties of monoclinic Ag_2S*, Mater. Chem. and Phys., 249, 122961 (2020).
34. X. Lu, Y. Liu, M. Shao and **X. Liu***, *Defect-mediated intercalation of dysprosium on buffer layer graphene supported by SiC(0001) substrate*, Chem. Phys. Lett., 742, 137162 (2020).
35. Y. Liu, **X. Liu,*** C.-Z. Wang, Y. Han, J. W. Evans, A. Lii-Rosales, M. C. Tringides, and P. A. Thiel, *Mechanism of Metal Intercalation under Graphene through Small Vacancy Defects*, J. Phys. Chem. C, 125, 6954−6962 (2021).
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