

## PUBLICATION LIST

1. **J. Xu**, P. Krüger, C. R. Natoli, K. Hayakawa, Ziyu Wu, and K. Hatada  
“X-ray absorption spectra of graphene and graphene oxide by full-potential multiple scattering calculations with self-consistent charge density”  
[Phys. Rev. B \*\*92\*\*, 125408 \(2015\)](#)  
My contribution: writing the paper, all calculations and code development
2. **J. Xu**, C. R. Natoli, P. Krüger, K. Hayakawa, Li Song, and K. Hatada  
“ES2MS: An interface package for passing self-consistent charge density and potential from Electronic Structure codes To Multiple Scattering codes”  
[Comp. Phys. Comm. \*\*203\*\*, 331 \(2016\)](#)  
My contribution: writing the paper, all calculations and code development
3. Q. Liu, X. Li, Z. Xiao, Y. Zhou, H. Chen, A. Khalil, T. Xiang, **J. Xu**, W. Chu, X. Wu, J. Yang, C. Wang,  
Y. Xiong, C. Jin, P. M. Ajayan, and L. Song  
“Stable Metallic 1T-WS<sub>2</sub> Nanoribbons Intercalated with Ammonia Ions: The Correlation between Structure and Electrical/Optical Properties”  
*Advanced Materials*, 2015, 27(33): 4837-4844  
My contribution: parts of first-principle simulations by VASP code
4. A. Marcelli, B. Spataro, S. Sarti, VA Dolgashev, S. Tantawi, DA Yeremian, Y. Higashi, R. Parodi,  
A. Notargiacomo, **J. Xu**, et al.  
“Characterization of thick conducting molybdenum films: Enhanced conductivity via thermal annealing”  
*Surface and Coatings Technology*, 2015, 261: 391-397  
My contribution: the analysis of X-Ray Diffraction data

## Manuscripts in preparation

1. **J. Xu**, K. Hatada, D. Sébilleau and Li Song  
“An efficient Multiple Scattering method based on partitioning of scattering matrix by angular momentum and approximations of matrix elements”  
<https://arxiv.org/abs/1604.04846>  
My contribution: writing the paper, all theory development, all code development and all calculations
2. D. Sébilleau, **J. Xu**, R. Choubisa, and C. R. Natoli  
“A complete multiple scattering approach to the EELS cross-section”  
My contribution: parts of the derivations of formulas

## Conference presentations

1. **J. Xu**, P. Krüger, C. R. Natoli, K. Hayakawa, Ziyu Wu, and K. Hatada  
“X-ray absorption spectra of graphene and graphene oxide by Full Potential Multiple Scattering calculations with self-consistent potential ”

**Oral**

The 16th International Conference on X-ray Absorption Fine Structure (XAFS16),  
Karlsruhe (Germany) (2015)

2. K. Hatada, **J. Xu**, K. Hayakawa, P. Krüger, and C. R. Natoli  
“Full Potential Multiple Scattering Theory with self-consistent charge and potential”

Poster

The 16th International Conference on X-ray Absorption Fine Structure (XAFS16),  
Karlsruhe (Germany) (2015)