

Introduction to Gaussian: Theory and Practice
Nanjing University, Nanjing, China
July 17 - 21, 2017



Day 1: Monday, July 17, 2017 - Chemistry Building H201

8:30	Registration	
9:00	Welcome & Computational Design	Lina Ding
9:30	Potential Energy Surfaces	Jingjing Zheng
10:00	Optimizing Reactants & Products	Lufeng Zou
10:30	Coffee Break	
11:00	Vibrational Spectroscopy & Thermochemistry	James Foresman
12:30	Lunch	

For the remainder of the workshop: NJU Teaching Center-Second Region-Gate 1

2:00	Laboratory I <ul style="list-style-type: none">• Welcome to GaussView• Building Molecules	
2:30	Wave Function Theory	Lufeng Zou
3:00	Basis Sets	Lina Ding
3:30	Input Files I	Douglas Fox
4:00	Coffee Break	
4:30	Laboratory II <ul style="list-style-type: none">• Running Electronic Structure Calculations I• Visualizing Spectra I	
6:30	Departure	

Day 2: Tuesday, July 18, 2017: NJU Teaching Center-Second Region-Gate 1

9:00	Optimizing Transition States	Jingjing Zheng
9:30	Electron Correlation	Douglas Fox
10:00	Reaction Path Following & Molecular Dynamics	Jingjing Zheng
10:30	Coffee Break	
11:00	Laboratory III <ul style="list-style-type: none">• Investigating Chemical Reactions I	
12:30	Lunch	
2:00	Density Functional Theory	Jingjing Zheng
2:30	Semi-Empirical & Molecular Mechanics Theories	Douglas Fox
3:00	Model Chemistry	James Foresman
3:45	Coffee Break	
4:15	Laboratory IV <ul style="list-style-type: none">• Analyzing Electronic Structure Results I• Visualizing Orbitals	
6:30	Departure	

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Day 3: Wednesday, July 19, 2017: NJU Teaching Center-Second Region-Gate 1

9:00	Solvation Models	Jingjing Zheng
9:30	ONIOM Hybrid Methods	Lufeng Zou
10:00	Nuclear Magnetic Resonance Spectroscopy	James Foresman
10:30	Coffee Break	
11:00	Laboratory V	
	<ul style="list-style-type: none"> • Gaussian Output • Investigating Chemical Reactions II 	
12:30	Lunch	
2:00	Optical & UV Spectroscopy	Lufeng Zou
2:30	Chiroptical Spectroscopy	Douglas Fox
3:15	Wavefunction & Orbital Analysis	James Foresman
3:45	Coffee Break	
4:15	Laboratory VI	
	<ul style="list-style-type: none"> • Visualizing Spectra II • Analyzing Electronic Structure Results II 	
6:30	Departure	

Day 4: Thursday, July 20, 2017: NJU Teaching Center-Second Region-Gate 1

9:00	SCF Problems & Strategies	Douglas Fox
9:45	Estimating Resource Requirements	Lufeng Zou
10:15	Coffee Break	
10:45	Laboratory VII	
	<ul style="list-style-type: none"> • From Gas to Solution Phase 	
12:30	Lunch	
3:30	Gaussian Input Files II	Lina Ding
4:00	Gaussian Utilities	James Foresman
4:30	Coffee Break	
5:00	Laboratory VIII	
	<ul style="list-style-type: none"> • Visualizing Spectra III 	
6:30	Departure	

Day 5: Friday July 21, 2017: NJU Teaching Center-Second Region-Gate 1

9:00	Complete Active Space Self-Consistent Field	James Foresman
9:30	Periodic Boundary Conditions	Douglas Fox
10:00	Coffee Break	
10:30	Summary	Lufeng Zou
11:00	Questions & Answers/Cleanup	All Instructors
12:30	Lunch & Departure	