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Type: Oral

Open Source Ion Dynamics Simulations - Challenges and Applications

Monday, August 25, 2025 2:10 PM (40 minutes)

Talk outline:

- Ion Dynamics, physical effects acting on ions:
- Coulombic Forces / Space charge
- Background Gas Collisions / Background Gas Interaction
- Ion Chemistry
- Current situation of ion dynamics simulation tools
- The case for open source tools
- Brief introduction of IDSimF
- Verification versus other Simulation tools
- FT-QIT: Space charge modeling
- basic problem: Quadratic scaling
- Barnes Hut approach
- FT-QIT: Experiment / Introduction
- IDSimF Simulation results
- Cl / Xe isotopes
- Space Charge Effects / Peak coalescence
- Space Charge Capacity
- Conclusio: Space Charge kills FT-QIT
- Similarly: Simple FT-LIT killed by space charge effects
- Ion Collisions / Collision Models:
- Hard Sphere Modeling as coarse approximation
- Molecular Dynamics Collision Model
- Basic approach
- Implementation in IDSimF
- Benchmark experiment:
- High Field IMS (HiKE)
- Simulation Results
- Challenges:
- Molecule Coalescence / Cluster Formation with Nitrogen
- Ion Chemistry:
- HiKE with water clusters

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