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A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS
INDEPENDENT UNIVERSITY OF MOSCOW

20-th V.A. Fock Meeting on Theoretical, Quantum and Computational Chemistry
26-30.08.2024,Novgorod,Russia

BOOK OF ABSTRACTS
of the 20-th V.A. Fock Meeting on Theoretical, Quantum and Computational Chemistry

A.L. Tchougréeff - Editor

Velikiy Novgorod

2024

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Tentative Schedule

"Life is richer than whatever scheme."

Monday August, 26th - Friday August, 30th

Time	Mon	Tue	Wed	Thu	Fri
10.00-11.00	Arrivals and Registration	Evarestov L 2437	Kvashnin L 2442	Zakharov L 2443	Tchougreeff L 2462
11.00-11.30		Coffee break	Coffee break	Coffee break	Coffee break
11.30-12.00		Pomogaeva O 2448	Turchenko O 2460	Raenko O 2461	Demin O 2452
12.00-14.00	Opening 13:45	Lunch	Lunch	Lunch	General Discussion and Closing
14.00-15.00	Ruette L 2435	Sabirov L 2440		Bezrukov L 2445	
15.00-15.30	Coffee break	Coffee break	Boat trip	Coffee break	Departures
15.30-16.00	Yuldasheva O 2438	Domnin O 2450		Sabirov O 2463	
16.00-16.30	Голованова O 2441	Prosnyak O 2453		Luscheev O 2464	
16.30-17.00					
17.00-17.30					
17.45-18.15	Welcome Party				
18.15-20.00			Conference Dinner		

EZFF2 – software for global optimization of force-field potentials: development of force-field potentials for modeling multi-walled WSe_2 nanotubes.

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The study presents a novel force field designed to model the properties of multi-walled nanotubes (MWNTs) composed of tungsten diselenide (WSe_2), addressing the limitations of ab initio methods for such large systems. Traditional quantum chemistry methods are computationally prohibitive for simulating MWNTs with experimentally relevant diameters. Thus, force field approaches remain essential, although many existing force fields are not optimized for MWNTs.

Using a gradient-free optimization algorithm, specifically the PSO [1], we calibrated the force field parameters to accurately reflect the properties of WSe_2 MWNTs. Our methodology involved computer tuning the force field to match a training set of experimental data and ab initio calculations for bulk phases, nanolayers, and single-walled nanotubes. The GULP [2] program was utilized for both force-field fitting and subsequent molecular mechanics or molecular dynamics simulations.

The developed force field was validated through comparisons with quantum chemical calculations and experimental data. Results indicate that the new force field accurately reproduces the structural and energetic properties of WSe_2 nanotubes, including interlayer distances and stability metrics. Notably, the interlayer interactions in WSe_2 contribute more significantly to nanotube stability than in WS_2, attributed to the larger and more polarizable selenium atoms.

Key findings include the successful simulation of the structure and stability of chiral and achiral MWNTs with diameters approaching experimental values. The force field's ability to predict properties of multi-walled nanotubes with various chirality angles and interlayer distances shows good agreement with experimental measurements.

This work underscores the potential of optimized force fields in modeling complex nanomaterials and provides a robust tool for future studies of WSe_2 MWNTs. Our findings pave the way for further theoretical exploration and potential experimental validation, contributing to advancements in nanoelectronics and optoelectronics.

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References:

1. Gad, A.G. Particle Swarm Optimization Algorithm and Its Applications: A Systematic Review. Arch Computat Methods Eng 2022, 29, 2531–256.
2. J. D. Gale, A. L. Rohl, Molec. Sim. 2003, 29 291-341.