Models for Simulation Based Selection of 3D Multilayered Graphene Biosensors

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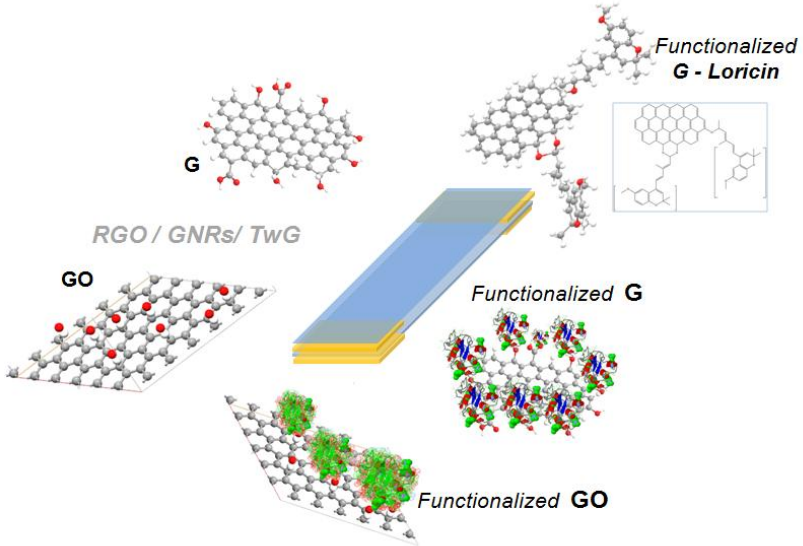
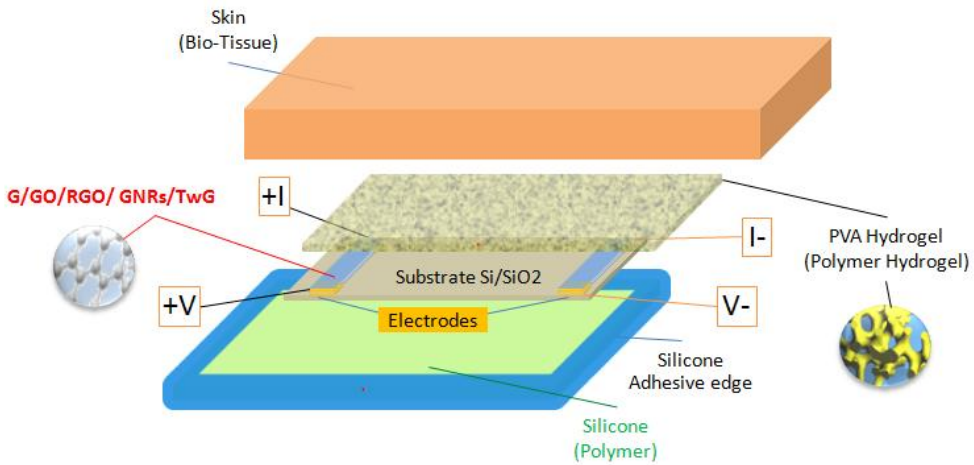
Overview

- Graphene biosensor models
- Density Functional Theory
- Graphene biosensor data
- Graphene models design & characterization (ChemBioOffice)
- Protein models design and characterization (ChemBioOffice)
- G/RGO/TwG Force Field characterization (MATLAB)
- Use of COMSOL Multiphysics
- COMSOL analysis: G-Biosensor structure model
- COMSOL analysis: Tween (TwG)- Biosensor structure model
- COMSOL Simulations (Acoustic Module): (TwG-E)/ SiO_2; SiO_2 -environment
- COMSOL Simulations (Acoustic Module):G/GO –SiO_2 interface
- Conclusions

Graphene biosensor models





Graphene (G), graphene oxides (GO), reactive graphene oxides (RGO), graphene nanoribbons (GNRs) and other graphene based composite materials (TwG) are used on the biosensing area with the aim of defining new functionalized material solutions for personalized medical applications.

Density Functional Theory

Lennard- Jones potential:

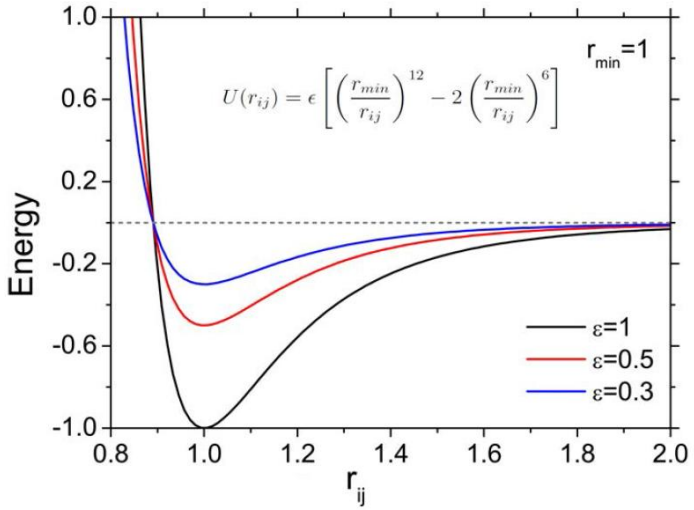
$$U(r_{ij}) = \epsilon \left[\left(\frac{r_{min}}{r_{ij}} \right)^{12} - 2 \left(\frac{r_{min}}{r_{ij}} \right)^{6} \right]$$

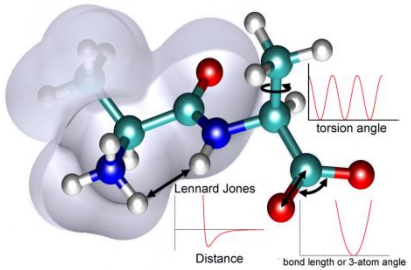
The force acting on the "*i*" atom of the system:

$$\vec{F}_i = -\frac{12\,\epsilon}{r_{min}^2} \sum_{\substack{j=1 \\ j \neq i}}^{N} \left[\left(\frac{r_{min}}{r_{ij}} \right)^{14} - \left(\frac{r_{min}}{r_{ij}} \right)^{8} \right] \vec{r}_{ij}$$

ϵ – the depth of the potential energy well [eV]

r_{min} –the distance at the minimum of the potential [A]





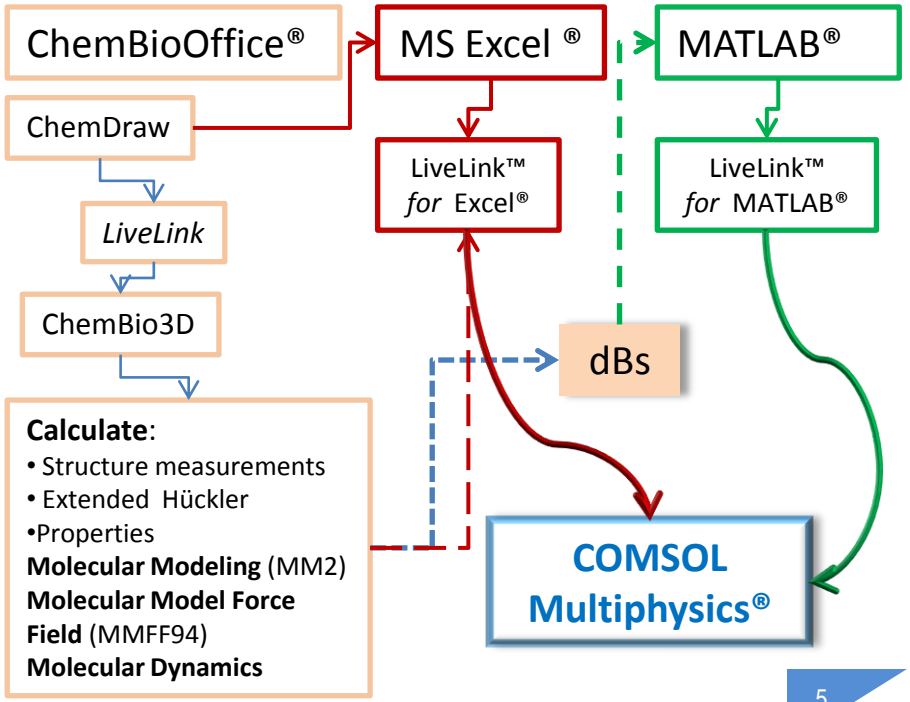
Parameters of **van der Waals** (vdW) interactions are specified through force field files *[Lennard-Jones potential dBs]*

Graphene biosensor data

Challenges

- **Design and characterization** - **graphene** (2D nano-structure): G, GO, RGO, etc
- **Design and characterization** – **bio-structure**: Alpha-Helix, Loricin, etc
- **Functional integration** :
  - human skin – hydrogel polymer structure (PVA Hydrogel);
  - PVA Hydrogel – graphene based module(G/GO/TwGP);
  - graphene module – electrodes (Ag);
  - graphene/electrodes – substrate (Silica glass SiO_2)
- **Device response** to environmental stimuli simulation

Modeling approach



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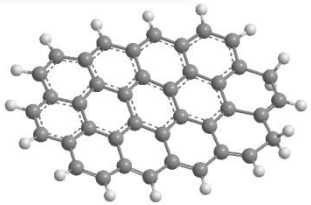
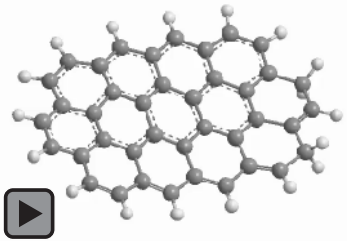
Graphene models design & characterization

Graphene G-H2

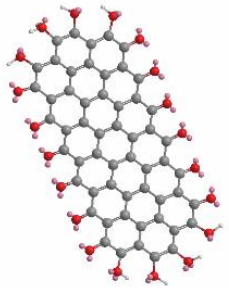


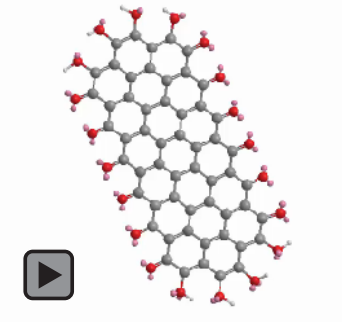


298.183 kcal/mol	**Total Energy of frame**	524.036 kcal/mol
31.222	**RMS gradient**	16.969
	Molecular Dynamics	
	Dynamics:	
2.0 fs	Step interval:	2.0 fs
10 fs	Frame interval:	10 fs
306 steps	Terminate after:	306 steps
1.000 kcal/atom/ps	Heating/Cooling Rate:	1.000 kcal/atom/ps
300 Kelvin	Target temperature:	300 Kelvin
	Properties:	
Exp →dB-Pi –BO_[G-H2]	Pi bond order	Exp →dB-Pi –BO_[G-OH]
Exp →dB-SEs_[G-H2]	Steric energy summary	Exp →dB-SEs_[G-OH]
	Extended Hückel	
	Calculate charges	
	Calculate surfaces	
209	**Iteration**	306
2.9399	**Stretch**	11.0341
1.7717	**Bend**	23.7161
0.0463	**Stretch-Bend**	0.5694
-82.6589	**Torsion**	28.8301
-8.4197	Non-1,4- vdW	-16.8827
59.1217	**1,4 vdW**	97.5110
0.0504	**Dipole/Dipole**	84.8992
-27.1485 kcal/mol	**Total Energy**	229.852 kcal/mol

Non 1,4 vdW – energy for the through-space interaction between pairs of atoms that are separated by more than three atoms
1,4 vdW – energy for the through-space interaction atoms separated by two atoms
MM2 – Molecular Mechanics
MMFF94 – Merck Molecular Force Field

Graphene G-OH





Protein models design & characterization

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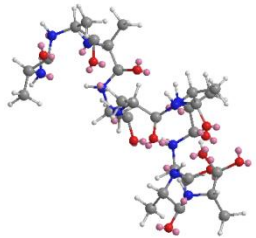
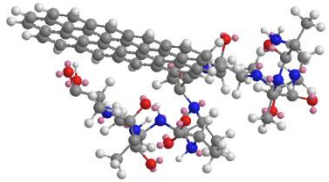
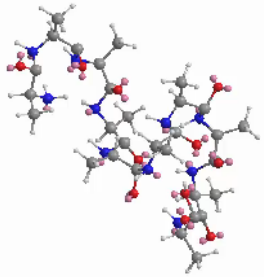
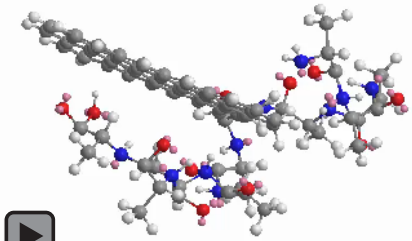
Functionalized Graphene-Protein assembly-design & characterization









-4.488 kcal/mol	**Total Energy of frame**	524.036 kcal/mol
6.4587	**RMS gradient**	16.969
	Molecular Dynamics	
	Dynamics:	
2.0 fs	Step interval:	2.0 fs
10 fs	Frame interval:	10 fs
1865 steps	Terminate after:	1494 steps
1.000 kcal/atom/ps	Heating/Cooling Rate:	1.000 kcal/atom/ps
300 Kelvin	Target temperature:	300 Kelvin
	Properties:	
Exp →dB-Pi –BO_[αHelix]	Pi bond order	Exp →dB-Pi –BO_[αHelix-G]
Exp →dB-SEs_[αHelix]	Steric energy summary	Exp →dB-SEs_[αHelix-G]
	Extended Hückel	
	Calculate charges	
	Calculate surfaces	
1865	**Iteration**	1494
1.9981	**Stretch**	4.7891
13.0319	**Bend**	13.2791
0.9841	**Stretch-Bend**	0.8170
6.0601	**Torsion**	-70.7286
-38.7740	Non-1,4- vdW	-68.6773
25.8378	**1,4 vdW**	85.5095
-13.6258	**Dipole/Dipole**	-7.3971
-4.4876 kcal/mol	**Total Energy**	-42.4084 kcal/mol

Non 1,4 vdW – energy for the through-space interaction between pairs of atoms that are separated by more than three atoms
1,4 vdW – energy for the through-space interaction atoms separated by two atoms
MM2 – Molecular Mechanics
MMFF94 – Merck Molecular Force Field

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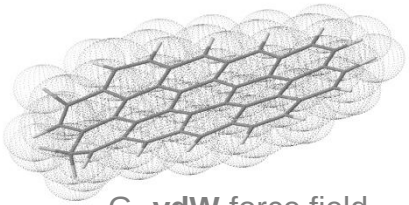
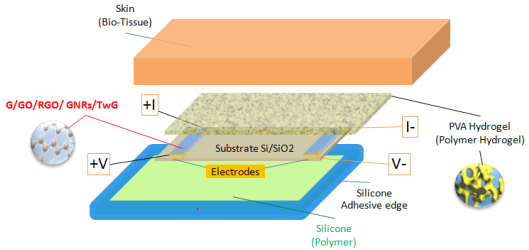
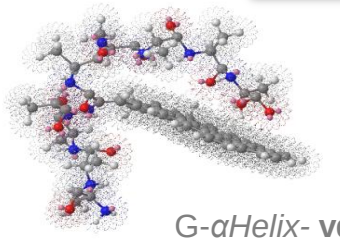
Van der Waals force field (DFT) assembly RGO/GNRs/TwG

Graphene models design & characterization

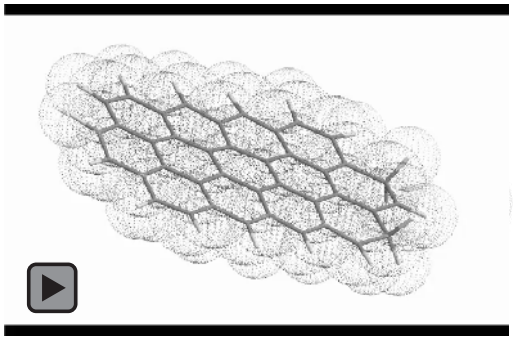


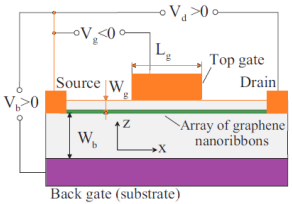
G- **vdW** force field

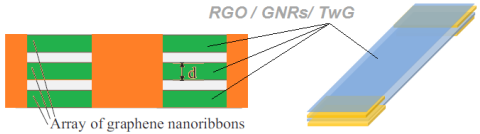


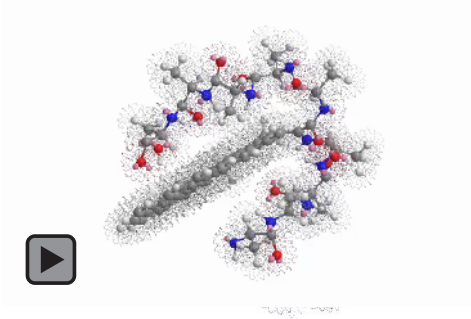


G-*αHelix*- **vdW** force field









G/RGO/GNRs/TwG
Force Field properties

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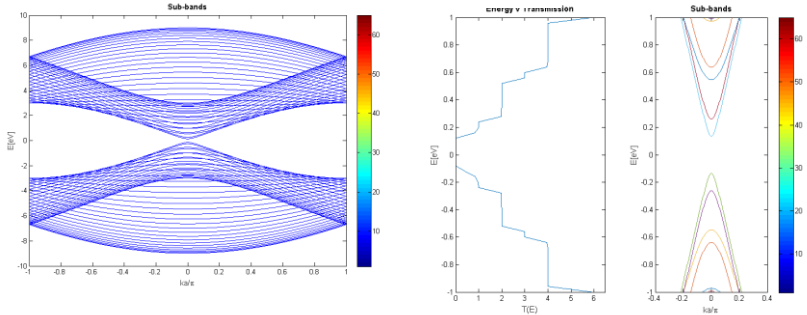
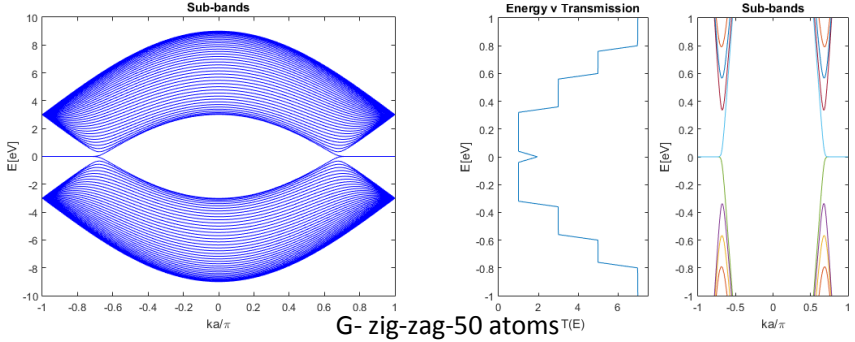
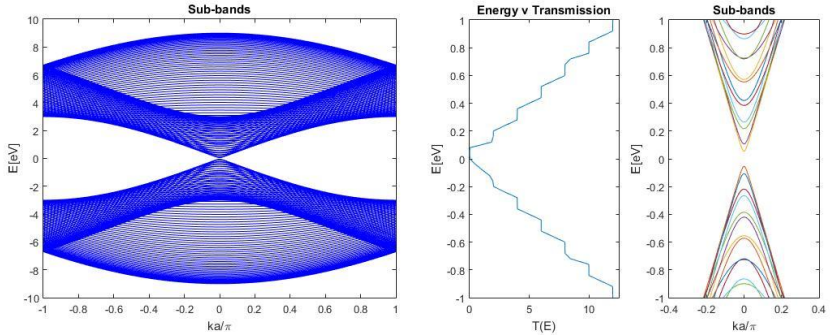
G- armchair-20 atoms



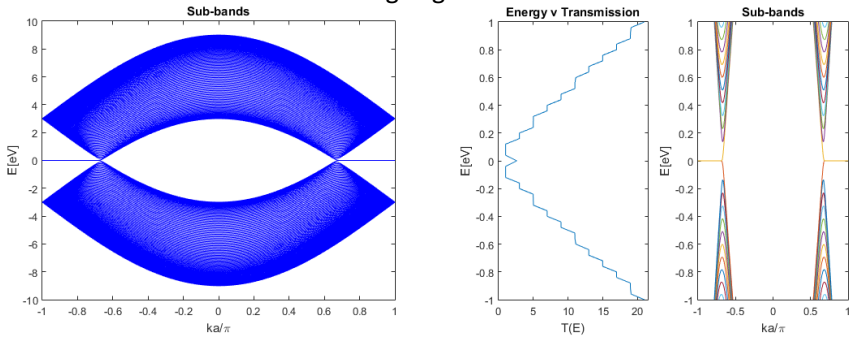
G- zig-zag-20 atoms



G- armchair-50 atoms



G- zig-zag-50 atoms



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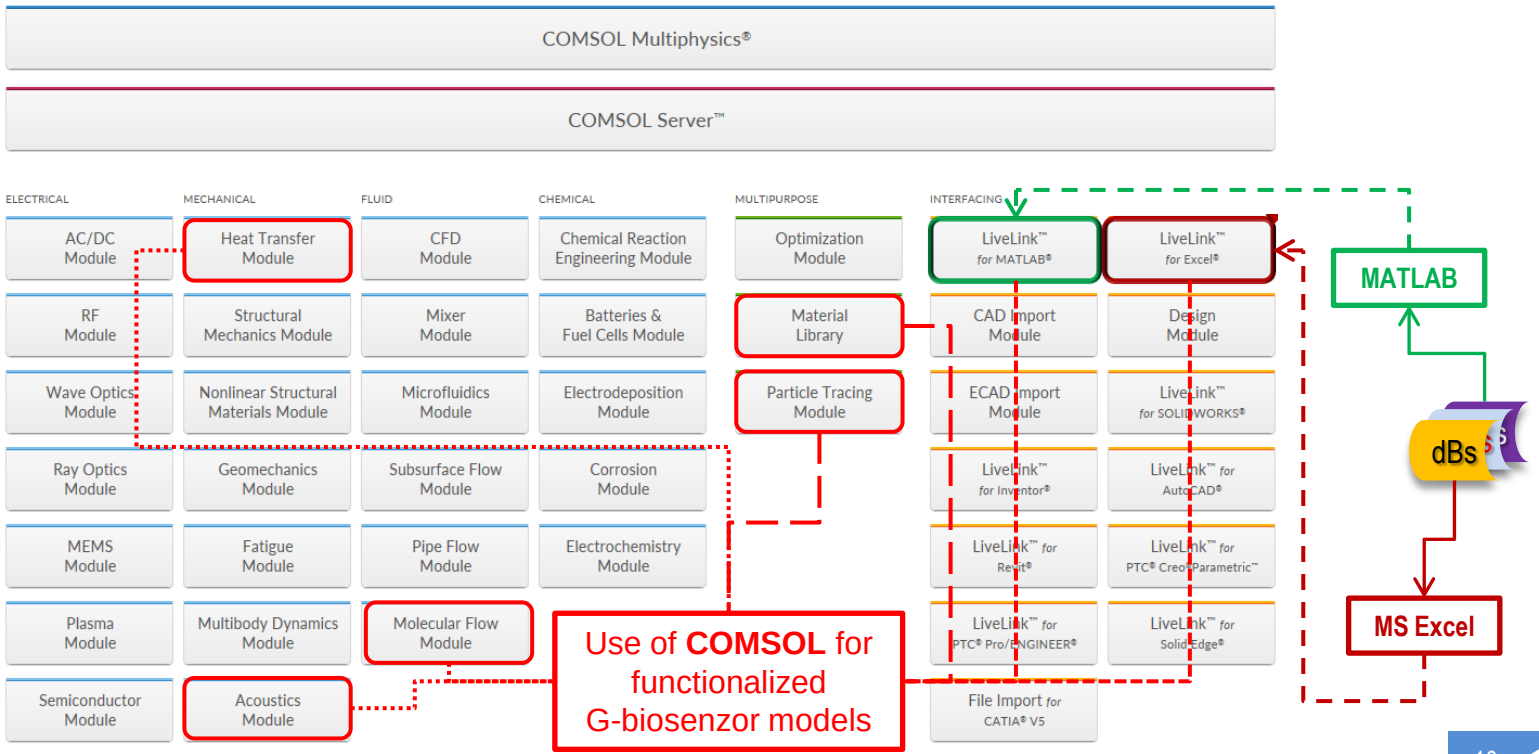
Use of COMSOL Multiphysics



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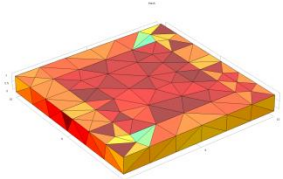
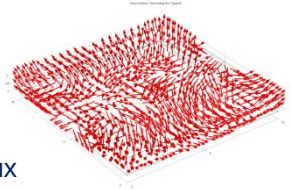
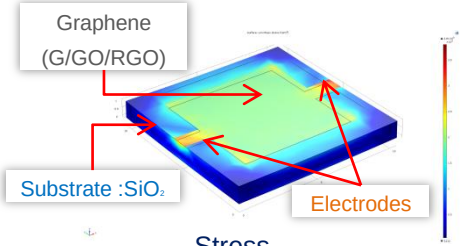
COMSOL analysis:
G-Biosensor structure model



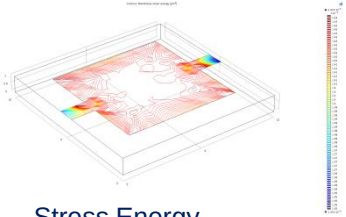
Mesh



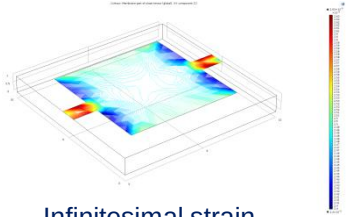
Energy Flux



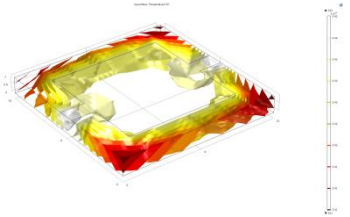
Stress



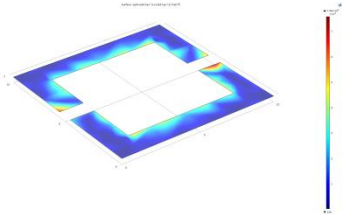
Stress Energy



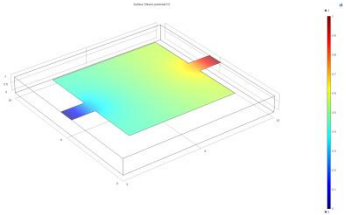
Infinitesimal strain tensor (G/GO/RGO)



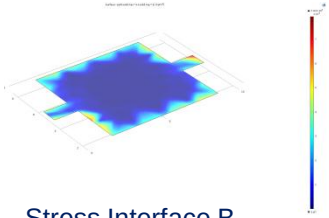
Isothermals



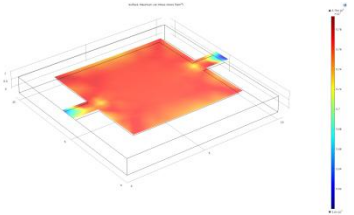
Stress Interface A



Electric Potential



Stress Interface B



Stress shell

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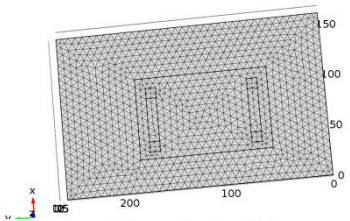
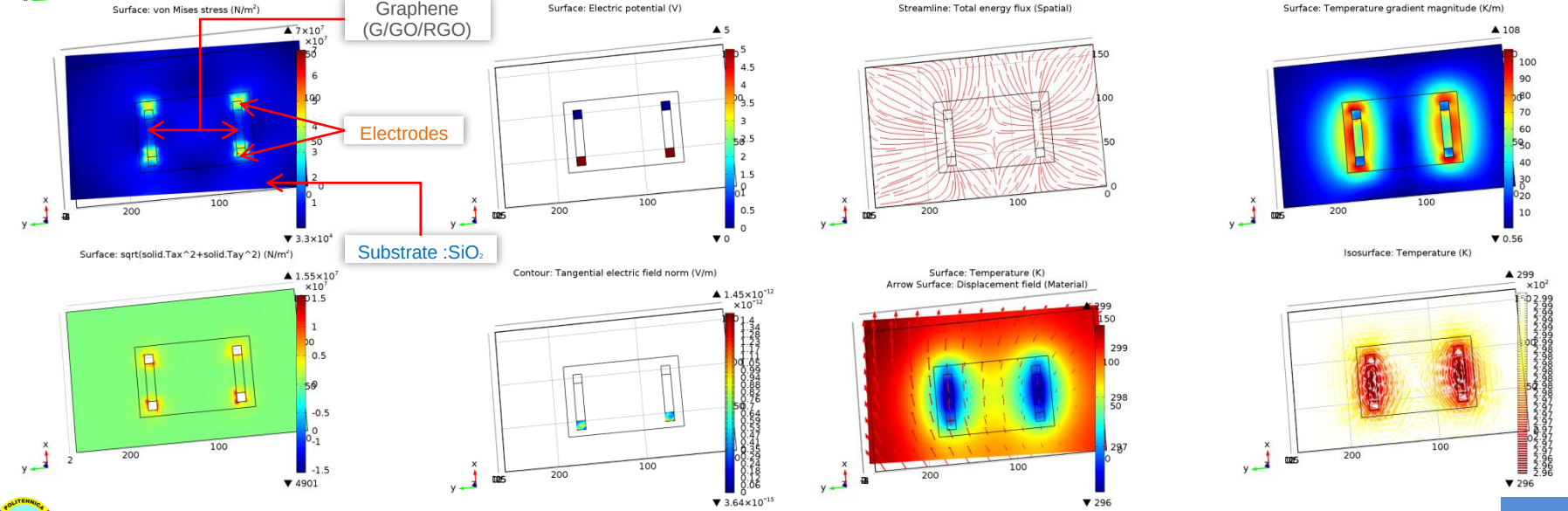
COMSOL analysis: Tween (TwG) - Biosensor structure model





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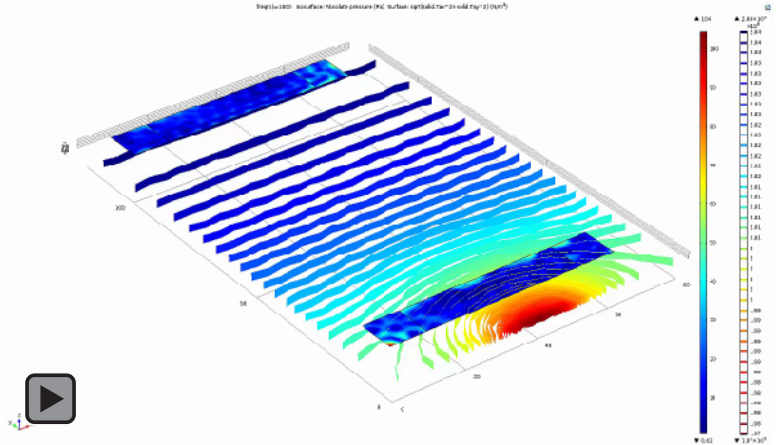
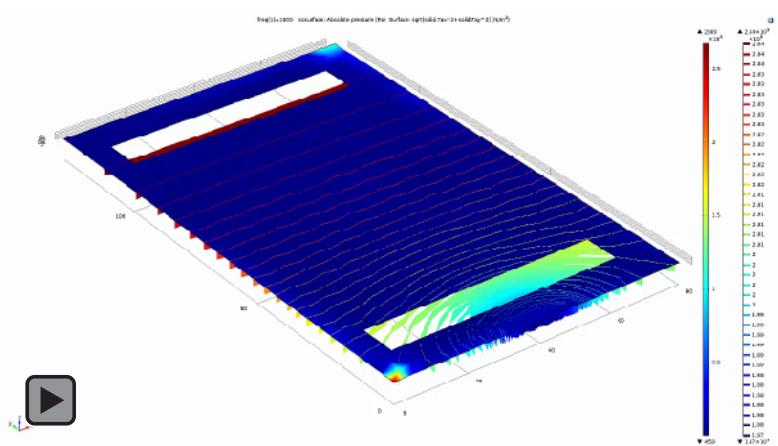
Simulating *interface responses* to environmental stimuli
GNRs- Electrode (TwG-E) /**Silicon Glass** (SiO_2)

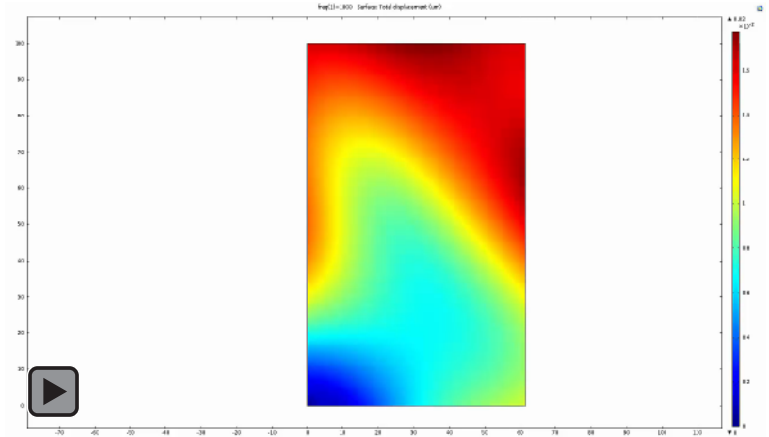


Simulating **Silicon glass** (SiO2)
response to environmental stimuli

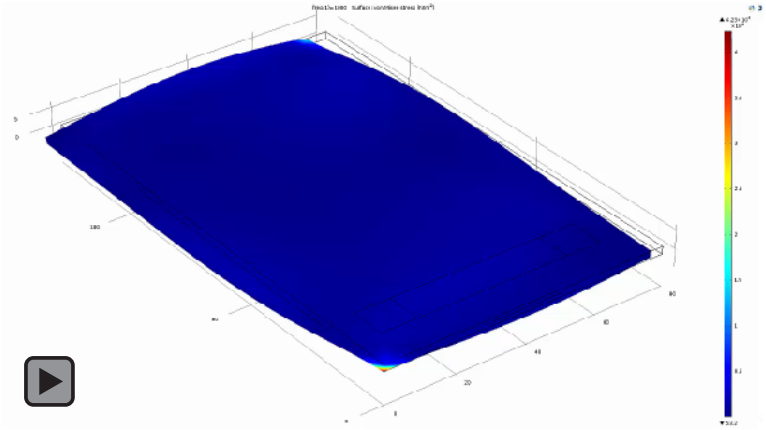


ChemBioOffice® MATLAB® **COMSOL**

Simulating **G/GO/RGO- SiO_2** module interface response to environmental stimuli



Simulating **G-protein-G** sandwich structure on **Silicon Glass** response to vibrations under environmental stimuli



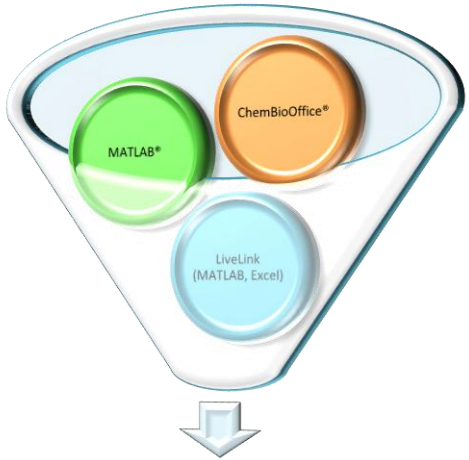
Conclusions

- Graphene *(G/GO/RGO/GNRs/TwG)* models, characterizations and field properties imported through LiveLink™ *(for Excel,and for MATLAB)* can be used for simulating graphene-biosensors' responses to environmental stimuli

- Van der Waals field forces potential *(based on: DFT, Lennard-Jones, Kirchhoff, and Frölich continuum)* applied for molecular and quantum level interactions *(electron-electron, phonon-phonon, electron-phonon)* can explain and simulate the G/GO/RGO-biosensing device continuum

- The functionalized G-protein-G structures, simulated as self-assembled structures, evolved during iterations towards stabile configurations *(DFT, vdW)*

- Biological and environmental stimuli *(thermal, electric, acoustic, chemical, etc)* are harvested by the functionalized graphene structures in continuum like models through the use of COMSOL Multiphysics modules



Questions?

Thank you!