Computational material discovery for gas sensing application

Hayk Zakaryan, Yerevan State University, hayk.zakaryan@ysu.am

Gas sensors applications:
- Medicine
- Food control
- Internet of Things
- Environment monitoring

Purposes and goals:
- Discovery of a new 2D material (transitional metal dichalcogenides).
- Simulate gas adsorption on the new 2D sensing material in room temperature.
- New methodology of investigation gas sensing materials for particular gases.

EYR support from ASNET-AM:
- More than 256 CPUs.
- About 1 TB memory.
- “Regional Workshop on Atomistic and Quantum Modelling”