Argonne NATIONAL LABORATORY

**Physical Science & Engineering / Computational, Environmental, & Life Sciences QIS Seminar**

PSE / CELS – QIS Seminar

# Igor Gayday

*Postdoctoral Fellow*

Marquette University

"Molecular Dynamics on Quantum Annealers"

Host: Stephen Gray

Monday, February 28, 2022
1:00 p.m.- 2:00 p.m.
ZoomGov Meeting ID 161 677 4612
Meeting Passcode: 337514
Join Meeting

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Abstract:

One of the most fundamental problems that has no efficient solutions on classical computers is simulation of quantum systems. It has been long hypothesized that quantum computing devices are naturally more suitable for this task, but many aspects of practical implementations of such simulations remain unknown. One particularly important kind of these simulations is the simulation of molecular dynamics, i.e. prediction of time evolution for a system of interacting particles. In this work we show how a quantum annealer can be used to carry out such simulations by solving differential equations of motion, on the example of the hydrogen molecule. Although the considered system is simple, our method is well scalable and can be readily applied to more complicated systems as annealers with larger number of qubits become available. Importantly, the method is general and can be used to solve arbitrary systems of ordinary non-linear differential equations, which can be helpful not only in the field of computational chemistry, but in many other fields as well.