

Dear Friends,

It is our pleasure to invite you to a half-day workshop “Fragment Molecular Orbital method” that will take place on Monday, August 15. The Fragment Molecular Orbital (FMO) method is the all-electron fragmentation technique that allows performing fully quantum ab initio calculations at molecular systems consisting of thousands of atoms (polymers, proteins, materials). The aim of the workshop is to provide participants with a theory background and hands-on experience in running and analyzing FMO calculations. The workshop will be led by the experts and developers of the FMO method, Dr. Dmitri Fedorov (Nanosystem Research Institute, AIST, Japan) and Dr. Yuri Alexeev (ANL).

FMO workshop, August 15, 1:00-5:30 pm, BRNG B291

1:00-2:00 pm - Theory of FMO method

2:00-3:00 pm - Practical course on modeling for FMO (FMOgen and FMOtools)

3:00-5:00 pm – Running and analyzing FMO calculations with GAMESS (using Facio and WinGAMESS)

5:00-5:30 pm - Q/A session

The BRNG B291 room is equipped with ITAP computers. However, if you prefer, you may bring and use your own laptop. In this case, please also bring a flash drive for easy transfer of the information. We will provide all necessary software.

Due to a limited space, we ask you to respond to Lyudmila Slipchenko lslipchenko@purdue.edu and let us know whether you plan to attend. We will accommodate the participants on the first-respond-first-serve basis.

