Computational analysis of methane occupation within gas hydrates PHILLIP MENDONCA, PHILIP SHEMELLA, SAROJ NAYAK, Department of Physics, Applied Physics, and Astronomy. Rensselaer Polytechnic Institute, ANURAG SHARMA, Department of Earth and Environmental Sciences. Rensselaer Polytechnic Institute — Gas hydrates are considered a future energy resource that have large quantities of hydrocarbon gases (mostly methane) trapped and stabilized under moderate pressures in continental shelf and permafrost regions. The global estimate of hydrocarbon stored in these ice-like structures far exceeds all fossil fuel reserves. Methane escape from these phases, therefore, is considered a potential global warming contributor. These characteristics make the gas hydrates energy recovery a technological challenge and requires constraining the methane diffusion process within the structure. Here, we present a first principles theoretical investigation into the structure, energetics and dynamics of the 'guest' molecule in gas hydrates, with the goal of building a physical model for methane diffusion. In particular, our study focuses on the sI (low pressure) methane hydrate phase by combining isolated cluster calculations and periodic structure calculations and closely guided by high pressure experimental work on methane hydrate. Based on the known crystal structure, we compare binding energies for methane and other gas molecules (e.g. Xe, Ar, CO_2) to guide the high pressure experiments.

Philip Shemella
Department of Physics, Applied Physics, and Astronomy
Rensselaer Polytechnic Institute