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**First-principles calculation of structural and electronic properties of memantine (Alzheimer's disease) and adamantane (anti-flu) drugs**[1]
KIRSTEN MIDDLETON, GUOPING ZHANG, Department of Physics, Indiana State University, THOMAS F. GEORGE, University of Missouri-St. Louis — Memantine is currently used as a treatment for mild to severe Alzheimer's disease, although its functionality is complicated. Using various density functional theory calculations and basis sets, we first examine memantine alone and then add ions which are present in the human body. This provides clues as to how the compound may react in the calcium ion channel, where it is believed to treat the disease. In order to understand the difference between calcium and magnesium ions interacting with memantine, we compute the electron affinity of each complex. We find that memantine is more strongly attracted to magnesium ions than calcium ions within the channel. By observing the HOMO-LUMO gap within memantine in comparison to adamantane, we find that memantine is more excitable than the anti-flu drug. We believe these factors to affect the efficiency of memantine as a treatment of Alzheimer's disease.

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