

CUTTING DIAMONDS IN THE ROUGH - TRAINING UNDERGRADUATES TO USE QM AND FREE ENERGY METHODS TO UNDERSTAND MOLECULAR BEHAVIOR

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Our research is diverse by design. We select projects for which the energetics and dynamical behavior of an interesting system are not well understood at the molecular level, the projects are manageable and attractive to undergraduate researchers even in their first or second year of study and the results of the projects will be of interest to the wider chemistry community, publishable and capable of attracting external grant support. Recent work describing the multireference character of benzyne diradicals, charge-transfer pathways of annulenes and conformational flexibility of potential HIV-fusion drug scaffolds will be described.