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Density functional theory investigation of cyclohexane as a potential functionalizing agent on graphene[1] CEREN SIBEL SAYIN, Department of Physics, Middle East Technical University, Ankara, Turkey, DANIELE TOFFOLI, Department of Chemistry, Middle East Technical University, Ankara, Turkey, HANDE ÜSTÜNEL, Department of Physics, Middle East Technical University, Ankara, Turkey — Single molecules can functionalize graphene both covalently and non-covalently for use in various applications. Their adsorption properties also become important in graphene-based catalysis. In this talk, we present density functional theory (DFT) results of the interaction of cyclohexane, cyclohexyl and cyclohexene with pristine and defected graphene. We investigate structural and electronic changes induced in graphene upon adsorption and explore the potentiality of graphene to be employed in the catalytic oxidation/hydrogenation of these molecules.

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