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# **Ultrasonic and bio-assisted synthesis of Ag@HNTs-T as a novel heterogeneous catalyst for the green synthesis of propargylamines: A combination of experimental and computational study**

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## **Abstract**

A novel heterogeneous catalyst is prepared through functionalization of halloysite nanotube with 1H-1,2,3-triazole-5-methanol and subsequent immobilization of silver nanoparticles through bio-assisted approach using *Arctiumplatylepis* extract. The resulting catalyst, Ag@HNTs-T, was characterized by using SEM/EDX, BET, XRD, FTIR, ICP-AES, TGA, DTGA and elemental mapping analysis. Moreover, we computationally assessed metal-ligand interactions in Ag@HNTs-T complex model to interpret the immobilization behavior of silver nanoparticles on HNTs surface via quantum chemistry computations. The catalytic activity of the catalyst was studied for the synthesis of propargylamines via A3 and KA2 coupling reactions under ultrasonic irradiation. The results demonstrated that Ag@HNTs-T could efficiently promote these reactions to furnish the corresponding products in high yields and short reaction times. The study of the recyclability of the catalyst and Ag(0) leaching confirmed that the catalyst was recyclability up to four reaction runs with slight Ag(0) leaching.

**Keywords:** A3 and KA2 coupling reactions, bio-synthesis, DFT and PCM calculations, halloysite, silver nanoparticles