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### Original Research Article

## A computational estimation for alkyl chain effect in Schiff base pyridinium fluoride ionic liquid on chemical reactivity, thermophysical properties, pharmacokinetics, and biological activity by DFT approach

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### ABSTRACT

In an attempt to develop the methodologies used for oil spill clean-up, polyurethane sponge was modified by deposition of NiFe<sub>2</sub>O<sub>4</sub> nanoparticles on the surface of the original polyurethane sponge under ultrasonic treatment. The fabrication process was facile and low-cost. The as-prepared magnetic sponge exhibited remarkable features including great porosity, high oil adsorption capacity, hydrophobicity, and reusability. In addition, the magnetic property of the modified sponge facilitated the process of oil-water separation. Indeed, the hydrophobicity of the modified sponge contributed to the adsorption of different types of oil and organic solvent on the sponge surface. The modified sponge exhibited the same characteristic peaks as those of the NiFe<sub>2</sub>O<sub>4</sub> magnetic nanoparticles, ascertaining the formation of the crystalline nickel ferrite nanoparticles. The XRD and FTIR results proved the formation of the composite. FESEM images of the nanocomposite showed a highly porous mulberry-like structure with a rough skeleton. More importantly, the oil and water contact angle measurements proved the hydrophobicity of the modified sponge.

**Keywords:** Polyurethane, oil adsorption, sponge, reusability, magnetic separation, NiFe<sub>2</sub>O<sub>4</sub> nanoparticles, oil removal