Study on Promising Adsorption Pairs from the Rigor of Thermodynamics and Surface Energy

タハミドウ, ハサン, ルポム

氏　　名　：TAHMID HASAN RUPAM
Name

論 文 名　：Study on Promising Adsorption Pairs from the Rigor of Thermodynamics and Surface Energy（厳密な熱力学と表面科学に基づく有望な吸着剤-吸着質ペアに関する研究）
Title

区　　分　：甲
Category

論 文 内 容 の 要 旨
Thesis Summary

With the conscious awareness regarding energy scarcity and ecofriendly energy conversion systems adsorption-based heat transformation systems have gained much popularity in recent times due their utilization of low-grade waste heat as driving energy. Gas adsorption onto solid porous materials finds its application in various technologies including but not limited to heat pumps, desiccators, desalination, atmospheric water harvesting, gas storage, gas sensing and separation and so on. One of the major drawbacks of the adsorption-based systems are them being bulky in size with a high installation cost. These drawbacks are mainly introduced due to lack of an optimum adsorbent material. Regardless of the application, the efficiency of any adsorption-based system largely depends on its isotherm and kinetics. To get the desired isotherm and sorption kinetics efforts have been made to modify the conventional adsorbents like silica gels, activated carbons, zeolites, etc. in various ways to get desired properties in the adsorbent material. Apart from that, emphasis is given on synthesizing different tailored porous materials like metal organic frameworks, aerogels, ionic liquids, etc. yet no clear break through is found in this particular research field. One of the reasons behi9nd this is the existing gap between the material science and the applied thermal engineering. This research gap predominantly depends on the existence of the state-of-the-art characterization techniques to relate the morphological characteristics of the adsorbent material with the adsorption phenomenon. Generally, adsorbent's BET surface area, pore size distribution, thermal/cycle stability, thermal conductivity etc. are correlated with the experimentally obtained adsorption isotherm and kinetics data to provide implicit indications for the scientists to understand the applicability of these adsorbents for their targeted systems. However, this

traditional characterization techniques do not incorporate any information about the surface chemistry of the adsorbent material. Additionally, these characterization techniques fail to address the reaction mechanism in molecular level between the adsorbent's surface and adsorbate molecule. Adsorption being a surface phenomenon is greatly influenced by the chemical properties of the adsorbent's surface. Therefore, keeping this research gap in mind, this thesis emphasizes on the total surface characterization (both morphological and chemical) of the various adsorbent materials with a view to correlating its surface energy properties with their respective adsorption isotherms and adsorption thermodynamics which will eventually reduce the gap between the material science and thermal engineering to an acceptable margin. This research stresses several key factors, firstly, it shows how adsorbent/adsorbate interaction can influence the adsorption thermodynamics. Secondly, it discusses on how the thermodynamic properties can be utilized in designing an optimum adsorbent material. After that, it shows how surface energy can influence the adsorption isotherms prior to how individual components of the surface energy effect the adsorption isotherms. Some of the notable outcomes of this thesis includes the thermodynamic characterization of some potential pairs for adsorption heat pump applications. The study revealed that AC/ethanol pairs are the most suited pairs for the chiller applications. Later, the Henry region adsorption isotherm for various potential AC/ethanol pairs were obtained experimentally. Using the Henry constant and near zero adsorption enthalpy the adsorbed phase entropy was modeled. Utilizing the adsorbed phase entropy and adsorbents' pore volume, a guideline was given for synthesizing optimum carbonaceous adsorbent for ethanol adsorption. Then focus was given on metal organic frameworks (MOFs) targeting water adsorption. Transitional metal doping was done on parent MOF to enhance its water sorption properties. The green synthesized samples showed higher values of SCE than the commercial one. Last but not the least, we selected three different MOFs- aluminum fumarate, MOF 801 and MIL 100 (Fe) and characterize their surfaces. We have showed the relation between the surface properties of adsorbents and the experimentally obtained adsorption isotherm.