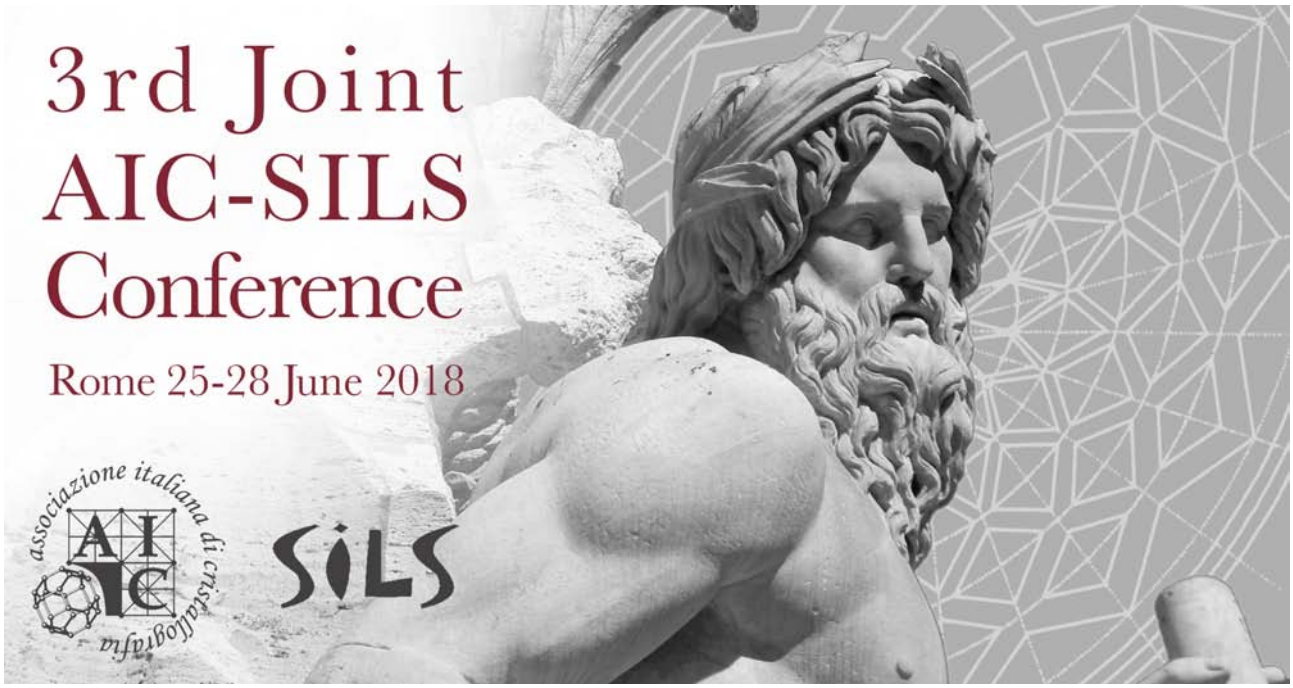

Programme and Book of Abstracts

3rd Joint AIC - SILS Conference - Rome 25-28 June 2018

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MS3 – KN1: New insight into the thermodynamic properties of high silica ZSM-5 zeolite: effect of adsorbed organic molecules

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High silica ZSM-5 zeolite compounds are known to experience a displacive monoclinic to orthorhombic (*m*↔*o*) phase transition at different transition temperatures depending on framework composition (*i.e.*, the Si/Al ratio), lattice defect density, as well as amount and physical-chemical properties of guest molecules. In detail, it has been shown that aggregates of twin domains of the monoclinic framework displace into an orthorhombic single crystal on increasing temperature, suggesting that the ZSM-5 monoclinic polymorph has the features of a ferroelastic material [1]. According to the Landau theory, the temperature evolution of an unloaded sample of ZSM-5 zeolite has been recently characterized through the analysis of the spontaneous strain variation revealing that the *m*↔*o* phase transition has a tricritical character [2]. Parallel investigations have demonstrated that hydrophobic ZSM-5 compounds possess physical properties (*e.g.*, high surface area, shape selectivity, and mechanical, thermal, biological, and chemical stability) that promote such compounds among those zeolites that are efficaciously employed in the adsorption processes of organic contaminants for wastewater treatments [*e.g.*, 3].
Although numerous works deal with the thermodynamic features of the *m*↔*o* ZSM-5 phase transition, the increasing interest in the scientific community on this compound employed as an efficient adsorbent perfectly matches with the lack of information on the thermodynamic processes operating when organic contaminants are adsorbed within the ZSM-5 zeolite structure.
The physical-chemical properties of guest molecules confined within a zeolite framework host are known to be strongly affected by the confinement effects exerted through noncovalent host-guest interactions. In this contribution, evidence for the strong coupling existing between the thermodynamic properties (enthalpy and entropy of adsorption) of organic molecules (such as, toluene, 1,2-dichloroethane, methyl-tert-butyl-ether, and their binary mixture) adsorbed within the ZSM-5 zeolite and the lattice strain driving the *m*↔*o* phase transition (ferroelastic-to-paraelastic) which controls connectivity and diffusivity in the zeolite framework is provided [4]. In particular, although the tricritical character of the *m*↔*o* phase transition is constant for all investigated compounds, it has been shown that the excess enthalpy part of the free-energy expansion (which derives from the coefficients of the Landau potential) is strictly related with the enthalpy of guest molecules adsorption.

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