To obtain accurate adsorption energies of molecules on surfaces is a challenging task as the methods with sufficient accuracy are too computationally demanding to be applied to the systems of interest. Embedding theories provide a natural remedy: focus the computation on a small region and incorporate the effects of the environment. In this thesis, embedding schemes and the response of many-electron systems to an adsorbed impurity are investigated. To this end, two approaches are used: tight-binding and ab initio. In the tight-binding method, the Green's function formalism is studied and explicit expressions for Green's functions of various one- and two-dimensional models are obtained. Using this formalism, we study qualitatively the local density of states and adsorption energies. In the second part of this thesis, state-of-the-art ab initio methods are employed to study convergence of the subtractive embedding scheme for adsorption energies of small closed-shell systems on two-dimensional graphene and hexagonal boron nitride. The efficiency and applicability of the scheme are assessed for neon and hydrogen fluoride as adsorbates. We found that the studied embedding method works better for neon compared to hydrogen fluoride, which may be explained by the use of a two-body dispersion correction.