Molecular separation with graphene nanowindows

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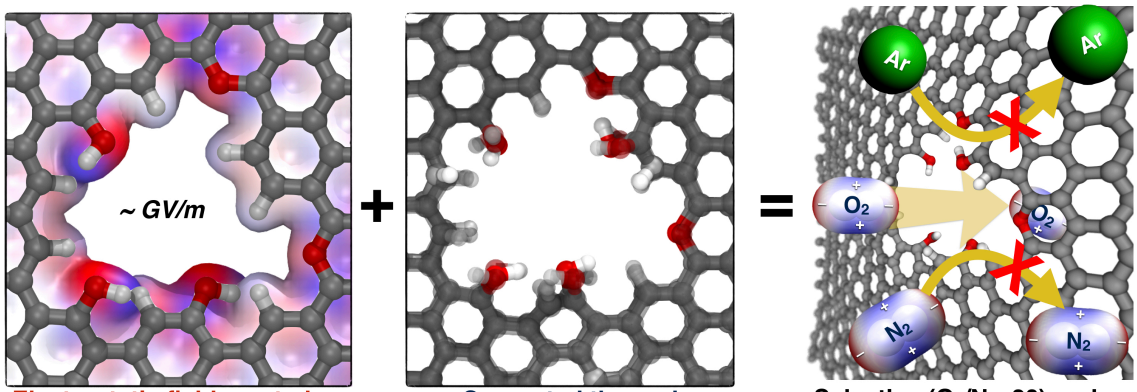
Graphene with nanoscale windows (nanowindows) can become the most selective, fastest and energy-efficient membrane for molecular separations. This nanowindow is not electrically neutral due to passivation of the carbon edges under ambient conditions, becoming a flexible atomic framework with functional groups along its rim. Through computer simulations of O_2, N_2 and Ar permeation, we reveal the remarkable nanowindow behavior at the atomic scale: (i) flexible nanowindows have thousand times higher permeability than conventional membranes and at least twice its selectivity. (ii) molecules 10% larger than a nanowindow easily permeate due to the concerted rim motion and short-lived transition state; (iii) an electrostatic field of GV/m order inside the nanowindow accelerates molecular permeation, and (iv) weakly interacting functional groups open/close the nanowindow to selectively control permeation. This selective ultra-fast permeation of O_2, N_2 and Ar in very restricted nanowindows contributes in designing the new generation of air separation membranes.

Graphene nanowindows are charged, flexible and selective



Reference:

Fernando Vallejos-Burgos, François-Xavier Coudert and Katsumi Kaneko (submitted, 2017).