

 [Print this Page for Your Records](#)[Close Window](#)**Control/Tracking Number:** 11-A-687-BPS**Activity:** Abstract**Current Date/Time:** 9/29/2010 3:47:49 PM**ACTIVE SITES OF ENZYMES ARE CROWDED WITH CHARGE****Author Block:** David Jimenez-Morales¹, JIE LIANG¹, BOB EISENBERG².¹University of Illinois at Chicago, Chicago, IL, USA, ²Rush Medical Center, Chicago, IL, USA.

Abstract: The chemistry of enzymes occurs at active sites that concentrate biological function into functional pockets. Functional pockets mix catalytic amino acids and substrate in tiny volumes. Here, we look for biological properties of that small space. We imagine that electric charge plays important roles, because even one charge in a small space produces large electric fields. To estimate densities of fixed charge, we measure the volume of functional pockets and count 'charged residues' in it. We collect locations of functional pockets from enzymes of known structure that catalyze the main six enzymatic reactions. Functional amino acids are identified by their participation in catalysis. We measure the volume of pockets using both solvent-accessible and molecular-surface models. 'Charged residues' are R, K and H (positive); E and D (negative). Charge density is extraordinarily large (~20 Molar on average, often larger). Mobile counterions for the fixed charge are presumably nearby in high density. Active sites do not resemble the infinitely dilute ideal solutions of classical enzyme kinetics. Their enormous charge density is comparable to the charge density of solid NaCl. Different types of enzymes have different charge densities. Hydrolases show the largest values of charge density. Some enzymes have extraordinarily large charge density -phosphoglycerate mutase (PDB = 1o98, density of charge 104 Molar, Molecular Surface), or sulfurtransferase (PDB = 1e0c, 109 Molar, Molecular Surface). Crowding of charged side-chains and ions produces enormous steric and electrostatic forces in these tiny active sites. The balance of these forces seems likely to be of great importance to enzyme function. Many charged pockets are also found away from active sites. Charged pockets are likely to be involved in many surface interactions. They may be reservoirs of electromechanical energy that can drive conformational changes.

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Author Disclosure Information: D. Jimenez-Morales: None. J. Liang: None. B. Eisenberg: None.

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* **Sponsor Email Address:** : beisenbe@rush.edu

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