## S.1 Figures



Fig A. ATP concentration profiles. Panels a)-c) represent uncharged systems with only a CD39 enzyme, in order of increasing junction radius, whereas d) is a solution for  $z_{ATP} = -2$  and  $\Phi_{junction} > 0$  and both CD39 and CD73 enzymes. The inset circles are the spherical inclusions representing the CD39 and/or CD73 enzymes. The spheres have a Dirichlet boundary condition of zero ATP concentration on their surface, resulting in a blue color in these images .



Fig B. Validation of solution to the electro-diffusion equation for a single enzyme under bulk-like conditions.  $k_{on,ATP}$  obtained from theoretical prediction (see Eq. 3 in Sect.) and simulation data for a bulk-like system with a single CD39 enzyme.



Fig C. Predictions of  $k_{on,ATP}$  as a function of junction/CD39 distance  $(d_{tether})$ , membrane potential and ionic strength ( $\kappa$ ). Note that for simplicity we assumed the linearized Poisson-Boltzmann equation here, thus the quantitative accuracy of the potentials > 25 mV is limited.



## Fig D. Efficiency of AMP to Ado conversion via CD39 and CD73

**catabolism.**  $k_{eff}$  values are reported for attractive versus repulsive junctional membrane potentials, degree of CD39/CD73 co-localization, and adjacency of the junctional membrane surface. All calculations assume  $z_{ATP}$ =-2,  $z_{AMP}$ =-1,  $z_{Ado}$ =0 and  $\Phi_{CD39} > 0$ .