

rearrangements and dehydration plays an important role in the selectivity process. It is suggested that conformational rearrangements can be caused by the lipid environment.

Acknowledgement

WBF thanks the Bionanotechnology IRC (Oxford) for financial support. Thanks also to A. Watts and J. Ryan (Oxford) for helpful discussions.

References and Footnotes

1. T. W. Allen, O. S. Andersen, and B. Roux. *Proc Natl Acad Sci USA* 101, 117-122 (2004).
2. T. W. Allen, and S. H. Chung. *Biochim Biophys Acta* 1515, 83-91 (2001).
3. A. Anishkin, and S. Sukharev. *Biophys J* 86, 2883-2895 (2004).
4. T. Bastug, P.-C. Chen, S. M. Patra, and S. Kuyucak. *J Chem Phys* 128, 155104-155109 (2008).
5. T. Bastug, A. Gray-Weale, S. M. Patra, and S. Kuyucak. *Biophys J* 90, 2285-2296 (2006).
6. A. T. Brünger. X-PLOR Version 3.1. *A System for X-ray Crystallography and NMR*. Yale University Press, New Haven, Ct. (1992).
7. A. E. Cardenas, R. D. Coalson, and M. G. Kurnikova. *Biophys J* 79, 80-93 (2000).
8. S.-H. Chung, M. Hoyles, T. Allen, and S. Kuyucak. *Biophys J* 75, 793-809 (1998).
9. E. A. Cohen, E. F. Terwilliger, J. G. Sodroski, and W. A. Haseltine. *Nature* 334, 532-534 (1988).
10. F. Cordes, A. Kukol, L. R. Forrest, I. T. Arkin, M. S. P. Sansom, and W. B. Fischer. *Biochim Biophys Acta* 1512, 291-298 (2001).
11. F. S. Cordes, A. Tustian, M. S. P. Sansom, A. Watts, and W. B. Fischer. *Biochemistry* 41, 7359-7365 (2002).
12. B. L. de Groot, and H. Grubmüller. *Science* 294, 2353-2357 (2001).
13. J. Deisenhofer, O. Epp, K. Miki, R. Huber, and H. Michel. *Nature* 318, 618-624 (1985).
14. J. T. Edsall, and H. A. McKenzie. *Adv Biophys* 10, 137-207 (1978).
15. G. D. Ewart, T. Sutherland, P. W. Gage, and G. B. Cox. *J Virol* 70, 7108-7115 (1996).
16. W. B. Fischer. *FEBS Lett* 552, 39-46 (2003).
17. D. Gillespie, W. Nonner, and R. S. Eisenberg. *J Phys: Condens Matter* 14, 12129-12145 (2002).
18. A. L. Grice, I. D. Kerr, and M. S. P. Sansom. *FEBS Lett* 405, 299-304 (1997).
19. H. Grubmüller, B. Heymann, and P. Tavan. *Science* 271, 997-999 (1996).
20. J. R. Gullingsrud, R. Braun, and K. Schulten. *J Comp Phys* 151, 190-211 (1999).
21. K. Heininger. Molecular dynamics simulations of aqueous systems. In *Computer Simulations of Fluids, Polymers and Solids*, p. 357. Eds., C. R. A. Catlow, S. C. Parker, and M. P. Allen. Kluwer Academic Publishers, Dordrecht (1990).
22. U. Hollerbach, D. P. Chen, D. D. Busath, and B. Eisenberg. *Langmuir* 16, 5509-5514 (2000).
23. H. Hwang, G. C. Schatz, and M. A. Ratner. *J Phys Chem B* 110, 26448-26460 (2006).
24. W. Im, S. Seefeld, and B. Roux. *Biophys J* 79, 788-801 (2000).
25. C. Jarzynski. *Phys Rev E* 56, 5018-5035 (1997).
26. C. Jarzynski. *Phys Rev E* 78, 2690-2693 (1997).
27. T. Klimkait, K. Strebel, M. D. Hoggan, M. A. Martin, and J. M. Orenstein. *J Virol* 64, 621-629 (1990).
28. V. Lemaitre, R. Ali, C. G. Kim, A. Watts, and W. B. Fischer. *FEBS Lett* 563, 75-81 (2004).
29. R. J. Leonard, C. G. Labarca, P. Charnet, N. Davidson, and H. A. Lester. *Science* 242, 1578-1581 (1988).
30. Z. W. Liu, Y. Xu, and P. Tang. *J Phys Chem B* 110, 12789-12795 (2006).
31. V. M. M. Lobo. *Pure Appl Chem* 65, 2613-2640 (1993).
32. H. Lu, B. Isralewitz, A. Krammer, V. Vogel, and K. Schulten. *Biophys J* 75, 662-671 (1998).
33. R. J. Mashl, Y. Tang, J. Schnitzer, and E. Jakobsson. *Biophys J* 81, 2473-2483 (2001).
34. T. Mehnert, Y. H. Lam, P. J. Judge, A. Routh, D. Fischer, A. Watts, and W. B. Fischer. *J Biomol Struct Dyn* 24, 589-596 (2007).
35. G. Moy, B. Corry, S. Kuyucak, and S. H. Chung. *Biophys J* 78, 2349-2363 (2000).
36. V. A. Parsegian. *Nature* 221, 844-846 (1969).
37. K. M. Ranatunga, I. D. Kerr, C. Adcock, G. R. Smith, and M. S. P. Sansom. *Biochim Biophys Acta* 1370, 1-7 (1998).
38. F. Revah, J. L. Galzi, J. Giraudat, P. Y. Haumont, F. Lederer, and J. P. Changeux. *PNAS USA* 87, 4675-4679 (1990).
39. B. Roux, S. Berneche, and W. Im. *Biochemistry* 39, 13295-13306 (2000).
40. B. Roux, and R. MacKinnon. *Science* 285, 100-102 (1999).
41. T. Schirmer, and P. S. Phale. *J Mol Biol* 294, 1159-1167 (1999).
42. U. Schubert, S. Bour, A. V. Ferrer-Montiel, M. Montal, F. Maldarelli, and K. Strebel. *J Virol* 70, 809-819 (1996).