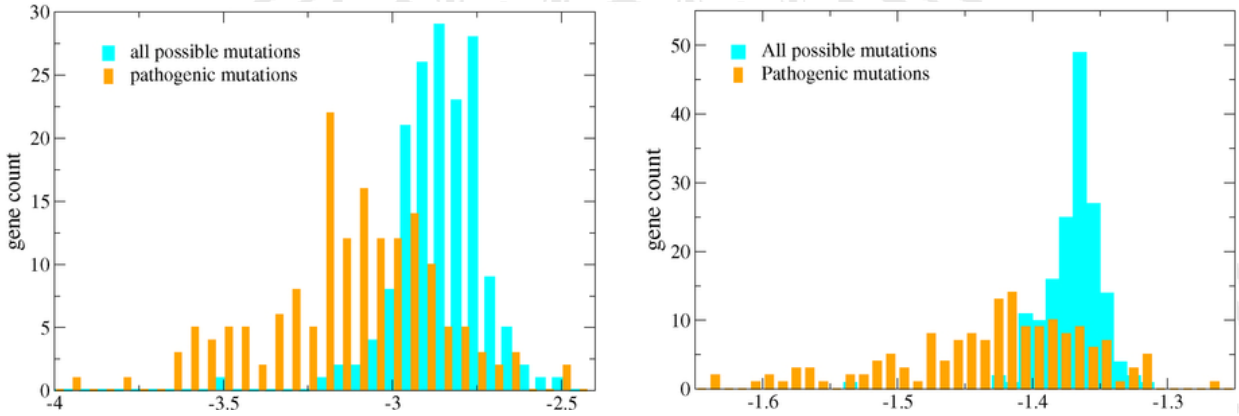
PHYSIKALISCHES KOLLOQUIUM

AM 23. JULI 2012 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



(c) **Distribution of change in charge transport for pathogenic (orange) and all (cyan) mutations.**

THE INTERPLAY OF MUTATIONS AND ELECTRONIC PROPERTIES IN DISEASE-RELATED GENES: A DOSE OF QUANTUM BIO-INFORMATICS

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Electronic properties of DNA are believed to play a crucial role in many phenomena in living organisms, for example the location of DNA lesions by base excision repair (BER) glycosylases and the regulation of tumor-suppressor genes such as p53 by detection of oxidative damage. However, the reproducible measurement and modelling of charge migration through DNA molecules at the nanometer scale remains a challenging and controversial subject even after more than a decade of intense efforts. Here we show [1], by analysing 162 disease-related genes from a variety of medical databases with a total of almost 20,000 observed pathogenic mutations, a significant difference in the electronic properties of the population of observed mutations compared to the set of all possible mutations. This correlation is novel, but not necessarily unexpected, as I will argue. As ours is inherently a statistical analysis, we have not been able to elucidate the causation behind the correlation. Even so, the knowledge that the change in electronic structure induced by mutations plays a role in fundamental biological and biochemical processes hints towards the possibility of electronic prediction, early diagnosis and detection of mutation hotspots.

[1] “The interplay of mutations and electronic properties in disease-related genes”, C-T Shih, SA Wells, C-L Hsu, Y-Y Cheng & RA Römer, Scientific Reports 2, 272 (2012)