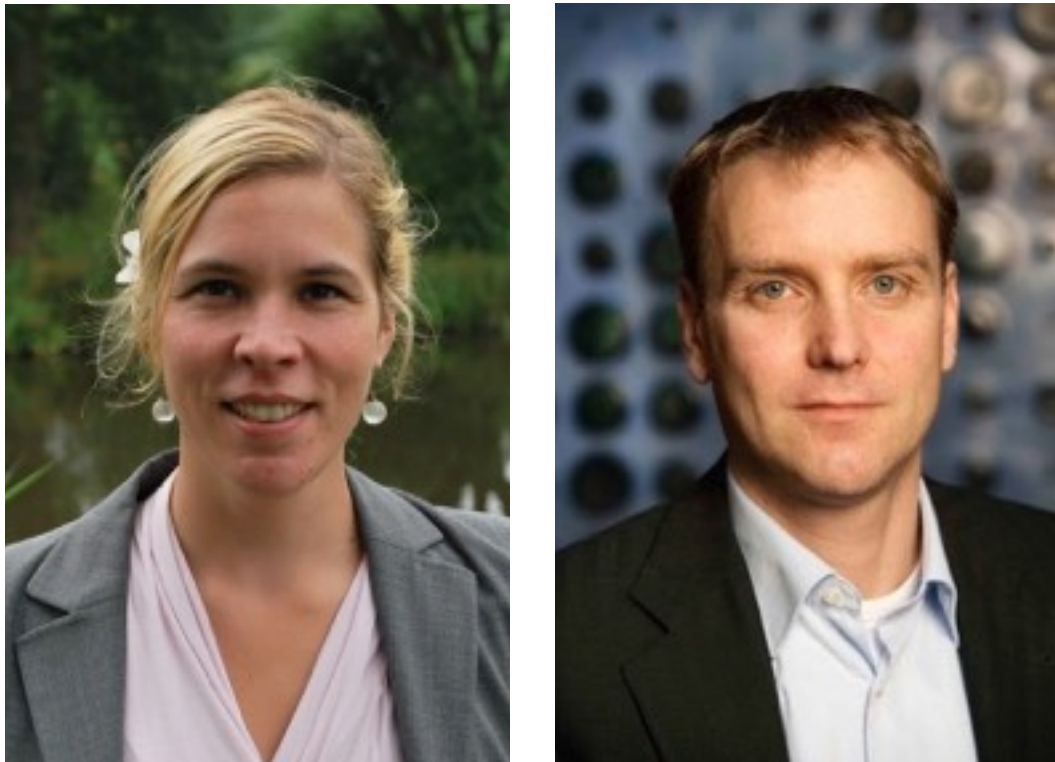


Conclusions

- ***Background:*** Hoogsteen base pairs are significant, and may play a role in biology
- ***Mechanisms:*** We see both the "inside" and "outside" mechanism, although there might be more preference for "outside"
- ***Rates and Free Energies:*** We overestimate the rates, but in a consistent manner. The free energy difference between the states is in very good agreement.
- ***Interesting remaining questions:***
 - Motions correlated with each of the mechanisms?
 - Role of specific sequence?
 - Paths based on leaving via minor groove?

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