# Effect of a nickel dimer on the dissociation dynamics of a hydrogen molecule

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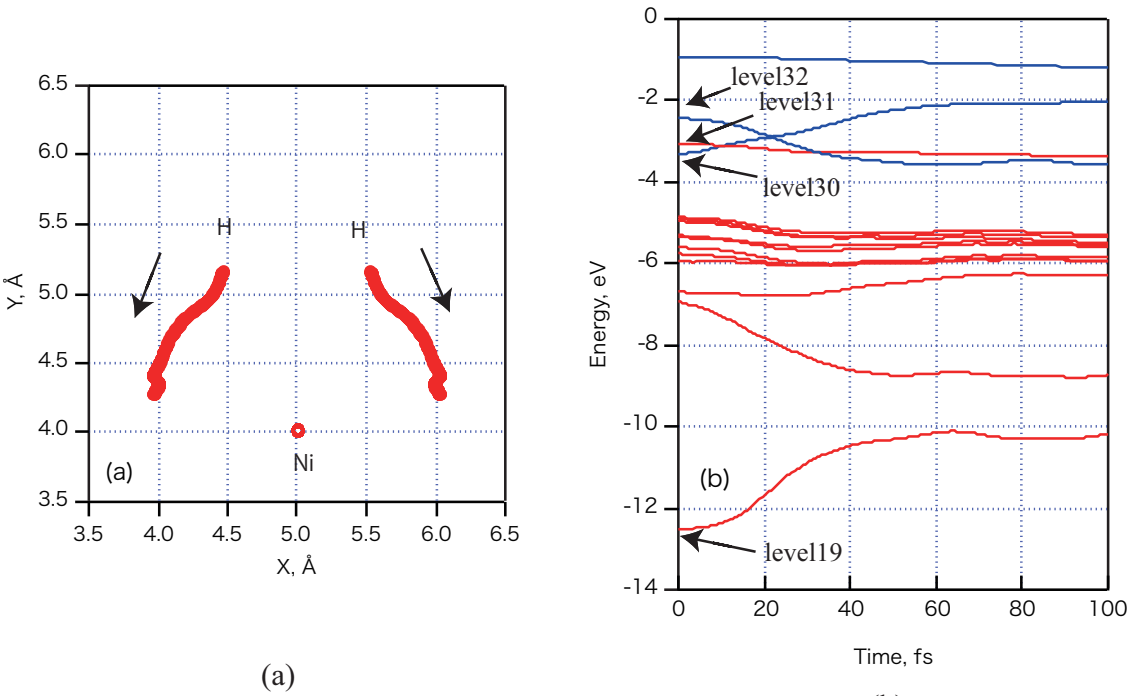
TOhoku Mixed Basis Orbitals *ab initio* program (TOMBO) which has been developed by our research group, where one electron wave functions are expressed by using both plane waves (PWs) and atomic orbitals (AOs) (1-2). One advantage of the program is that by combining AOs with PWs all-electron calculations can be performed very accurately with a modest computational cost. Properties associated with core levels, e.g. hyperfine structure constant, high speed collision of atoms can be accurately and efficiently computed with the modest computational effort.

As an example, a possibility of dissociation of a hydrogen molecule around a nickel dimer is investigated as a simple example of the initial stage of the hydrogen spill-over process(3). The electron and the ion dynamics are analyzed employing Ehrenfest's theorem and solving the time-dependent Kohn-Sham equation of time-dependent density functional theory coupled with the Newtonian equation of motion. The hydrogen molecule starts to dissociate under one electron excitation from the highest occupied molecular orbital level to the lowest unoccupied molecular orbital level (see Fig.1), while the exited electron level crosses the lower hole level yielding an energy gain. It is seen that the actual activation energy needed for this hydrogen dissociation process is reduced to only 0.10 eV, which is only possible in the presence of the nickel dimer. While without the nickel dimer dissociation requires a much larger excitation energy, well beyond that available from thermal fluctuations. This clearly shows the catalytic effect of the nickel dimer on the $H_2$ dissociation.




(a) (b)

Figure1 (a) The trajectory of hydrogen atoms of a hydrogen molecule around a nickel dimer (pointing perpendicular to the figure plane) when one (up-spin) electron is excited from the HOMO level to the LUMO level. (b) The time evolution of the energy levels.

References:

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[2] M. S. Bahramy, M. Sluiter, and Y. Kawazoe, Phys. Rev. B 73, 045111 (2006).

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