Selective control of photoassociation of Yb2: by theoretical study

Junxia Cheng[1], Hong Zhang[2], Xinlu Cheng[2], Jia Wang[1], and Shenjiang Wu[1]

[1]Xi'an Technological University
[2]Sichuan University

August 18, 2020

Abstract

The selective control of photoassociation of Yb2 molecule is investigated in theory. Based on ab initio to rationalize Franck-Condon filtering, the optimal target states of photoassociation have been obtained. That correspond to vibrational transition levels from X1Σ+g to excited state (A1Σu+, B1Πu , C1Σu+, D1Πu) are v'=23, 50, 55, and 0, respectively. The proposed laser drive transitions to target states for association process at wavelength A1Σu+: 464.7nm, B1Πu: 373.1nm, C1Σu+: 361.8nm, D1Πu: 339.1nm are determined. By using quantum wave-packet dynamic methods, we calculated the yields with time evaluation for the selected target states. Interacting with a resonant laser pulse, the projections of time-dependent wave functions of initial states on the target vibrational eigenstates reflected the photoassociation yields of Yb2. For target A1Σu+, using gaussian pulse made the value of v'=23 up to 97% at 725fs. After a laser pulse, that the positive chirp promotes the yield of projection of vibrational states to increase, but the negative chirp inhibits it decrease. For D1Πu state, when laser intensity is 1.0×1014 W/cm2, not only the purity is high but also the yield is high reached 99% of target state v'=0 at 1570fs. That is to say, by changing the laser parameters and pulse shapes, it could much easier control the photochemical along our desired direction. These conditions will provide an important reference and suggest a scheme for a feasible photoassociation for further experimental and theoretical researches.

Hosted file

`manuscript.doc` available at https://authorea.com/users/351849/articles/476304-selective-control-of-photoassociation-of-yb2-by-theoretical-study