# Quiz 2 (50 mins)

**Quiz Rules**

1. You are expected to abide by highest standards of academic honesty. You have been apprised of it during the first lecture.
2. State the assumptions made very clearly.
3. You are allowed to carry calculator and pen.
4. *Above all, read the question carefully.*

1. [100 points] One of the processes for hydrogen production is the water-gas shift reaction ($CO + H_2O \longrightarrow CO_2 + H_2$). Accurate density functional theory calculations predicts that the mechanism for water gas shift reaction is given by:

   (a) $CO + S \rightleftharpoons CO{\cdot}S$
   (b) $H_2O + S \rightleftharpoons H_2O{\cdot}S$
   (c) $H_2O{\cdot}S + S \rightleftharpoons OH{\cdot}S + H{\cdot}S$
   (d) $OH{\cdot}S + CO{\cdot}S \rightleftharpoons CO_2{\cdot}S + H{\cdot}S$
   (e) $CO_2{\cdot}S \rightleftharpoons CO_2 + S$
   (f) $2\,H{\cdot}S \rightleftharpoons H_2 + 2\,S$

   Further, in-situ spectroscopic measurements have shown that under the reaction conditions the surface is mostly covered with CO and H.

   Derive a rate expression assuming that step (d) is the irreversible rate-determining step, and all other steps are in quasi-equilibrium.

   Derive another rate equation assuming that water dissociation is the irreversible rate-determining step and all other steps are in quasi-equilibrium.

   Experimental data at constant water concentration has been reported suggesting that the reaction orders are 0.6 and -0.6 with respect to CO and $H_2$ respectively. Does any of the above rate expression consistent with the experimental data?