# Supplementary material for "Efficient and accurate description of adsorption in zeolites

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## I. PAW POTENTIALS USED

The details describing the standard and hard PAW potentials are listed in Table S1.

## II. INPUTS

The structures used for the calculations are stored in a separate file `structures.tar.gz` in the root directory of SI.

The input files are stored in file `incars.tar.gz`, one directory with inputs for MP2 calculations, second for RPA calculations. The directory also cotains a file `script_part.sh` which lists part of the script that was used to run the calculations.

TABLE S1. The details of the PAW potentials used in this study. We give the name and date of creation as stated in the file together with the number of projectors and the cut-off radius for the $s$ angular momentum projectors. Finally, the recommended plane-wave basis-set cut-off energy $E_{\mathrm{cut}}^{\mathrm{pw}}$ (`ENMAX` in POTCAR) is also given.

| Atom | Name | Date | $N_s$ | $r_s$ | $E_{\mathrm{cut}}$ |
|---|---|---|---|---|---|
| | | Standard | | | |
| H | H_GW | 21Apr2008 | 2 | 0.95 | 300 |
| C | C_GW | 28Sep2005 | 2 | 1.2 | 414 |
| O | O_GW | 28Sep2005 | 2 | 1.2 | 415 |
| Si | Si_GW | 04May2012 | 2 | 1.9 | 245 |
| Al | Al_GW | 19Mar2012 | 2 | 1.9 | 240 |
| | | Hard | | | |
| H | H_h_GW | 21Apr2008 | 2 | 0.8 | 700 |
| C | C_h_GW | 23May2013 | 3 | 1.0 | 742 |
| O | O_h_GW | 22May2013 | 3 | 1.0 | 766 |
| Si | Si_sv_GW_nc | 03Jul2013 | 3 | 1.70 | 610 |
| Al | Al_sv_GW_nc | 03Jul2013 | 3 | 1.75 | 572 |