

# Rendering all semiconductor **bandgaps** as a $\text{\LaTeX}$ table

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This package presents the position (potential) of the valence and conduction band edges for semiconductors in contact with an aqueous electrolyte as an R dataframe. The package was created mainly to make it easier to use and share this dataset (which is entirely based on primary literature sources). Apart from the included data, the package contains a number of auxiliary functions meant to i) add new data, ii) tabulate the data, and iii) plot the band edges visually.

In this vignette we demonstrate how the included data (`bandgaps::semiconductors`) can be typeset using  $\text{\LaTeX}$  (see table 1). To make the rendered table look pretty, we will compress some columns and display comments as tabular footnotes, but without removing any data from display.

We will render the table using `xtable` (that chunk is shown at the end of this document).

## Nernstian pH dependence

For many semiconductors in aqueous solutions,  $\text{H}^+$  and  $\text{OH}^-$  are the dominant adsorbed species, and therefore the potential drop across the Helmholtz layer,  $V_{\text{H}}$ , and the flatband potential changes systematically with pH. The potential of zero  $\zeta$  potential (PZZP, also known as the point of zero charge, PZP) is the pH at which the potential drop across the Helmholtz layer is zero [5]. The change of  $V_{\text{H}}$  with pH follows a straight-forward Nernstian relationship:

$$V_{\text{H}}/V = 0.059 \text{ V}(\text{pH}_{\text{PZC}} - \text{pH}) \quad (1)$$

I will assume that all oxides in this dataset obey this Nernstian pH dependence. As for sulfides, literature reports are conflicted on the matter, [5, 7] so out of an abundance of caution we will treat all sulfides as non-Nernstian. In some cases, individual non-oxide semiconductors have been shown to follow Nernstian pH behaviour. To keep track of Nernstian (or not) behaviour for all semiconductors, we have added a boolean variable `Nernstian` to the dataset (either `TRUE` or `FALSE`).

## References

- [1] Shelly Burnside et al. “Nanocrystalline Mesoporous Strontium Titanate as Photoelectrode Material for Photosensitized Solar Devices: Increasing Photovoltage through Flatband Potential Engineering”. In: *The Journal of Physical Chemistry B* 103.43 (Oct. 1999), pp. 9328–9332. ISSN: 1520-6106. DOI: 10.1021/jp9913867.
- [2] Sheng-Cheng Chiu and Yuan-Yao Li. “SiC Nanowires in Large Quantities: Synthesis, Band Gap Characterization, and Photoluminescence Properties”. In: *Journal of Crystal Growth* 311.4 (Feb. 2009), pp. 1036–1041. ISSN: 00220248. DOI: 10.1016/j.jcrysgro.2008.11.099.
- [3] Wang-Jae Chun et al. “Conduction and Valence Band Positions of  $\text{Ta}_2\text{O}_5$ ,  $\text{TaON}$ , and  $\text{Ta}_3\text{N}_5$  by UPS and Electrochemical Methods”. In: *The Journal of Physical Chemistry B* 107.8 (Feb. 2003), pp. 1798–1803. ISSN: 1520-6106. DOI: 10.1021/jp027593f.
- [4] Di Liu and Prashant V. Kamat. “Photoelectrochemical Behavior of Thin  $\text{CdSe}$  and Coupled  $\text{TiO}_2/\text{CdSe}$  Semiconductor Films”. In: *The Journal of Physical Chemistry* 97.41 (Oct. 1993), pp. 10769–10773. ISSN: 0022-3654. DOI: 10.1021/j100143a041.
- [5] Arthur J. Nozik. “Photoelectrochemistry: Applications to Solar Energy Conversion”. In: *Annual Review of Physical Chemistry* 29.1 (Oct. 1978), pp. 189–222. ISSN: 0066-426X. DOI: 10.1146/annurev.pc.29.100178.001201.
- [6] W. H. Strehlow and E. L. Cook. “Compilation of Energy Band Gaps in Elemental and Binary Compound Semiconductors and Insulators”. In: *Journal of Physical and Chemical Reference Data* 2.1 (1973), p. 163. ISSN: 00472689. DOI: 10.1063/1.3253115.
- [7] Yong Xu and Martin A. A. Schoonen. “The Absolute Energy Positions of Conduction and Valence Bands of Selected Semiconducting Minerals”. In: *American Mineralogist* 85.3-4 (2000), pp. 543–556. DOI: 10.2138/am-2000-0416.

**Table 1** Band edge levels at the pH of ZPC for each material. All band edge potentials vs SHE at the given pH for each semiconductor. The point of zero surface charge for each material is given (where available) in the column labelled pH<sub>ZPC</sub>.

Formula	Class	$E_{CB}/V$ vs SHE	$E_{VB}/V$ vs SHE	$E_g/V$	pH	pH <sub>ZPC</sub>	Ref	Note
ZrO <sub>2</sub>	oxide	-1.03	3.97	5.00	6.70	6.7	[7]	
Ta <sub>2</sub> O <sub>5</sub>	oxide	-0.11	3.89	4.00	2.90	2.9	[7]	
ZnS	sulfide	-0.98	2.62	3.60	1.70	1.7	[7]	
SnO <sub>2</sub>	oxide	0.06	3.56	3.50	4.30	4.3	[7]	
NiO	oxide	-0.44	3.06	3.50	10.30	10.3	[7]	
KTaO <sub>3</sub>	oxide	-0.87	2.63	3.50	8.55	8.55	[7]	
SrTiO <sub>3</sub>	oxide	-1.20	2.20	3.40	8.60	8.6	[7]	
BaTiO <sub>3</sub>	oxide	0.14	3.44	3.30	9.00	9	[7]	
<i>n</i> -TiO <sub>2</sub> (anatase)	oxide	-0.23	2.97	3.20	5.80	5.8	[7]	
ZnO	oxide	-0.25	2.95	3.20	8.80	8.8	[7]	
<i>n</i> -TiO <sub>2</sub> (rutile)	oxide	-0.76	2.24	3.00	13.00	NA	[1]	
CuTiO <sub>3</sub>	oxide	-0.12	2.87	2.99	7.29	7.29	[7]	
FeTiO <sub>3</sub>	oxide	-0.15	2.65	2.80	6.30	6.3	[7]	
SiC	carbide	-0.46	2.34	2.80	14.00	NA	[2]	<sup>1</sup>
In <sub>2</sub> O <sub>3</sub>	oxide	-0.56	2.24	2.80	8.64	8.64	[7]	
WO <sub>3</sub>	oxide	0.80	3.50	2.70	0.43	0.43	[7]	
<i>n</i> -TaON	oxynitride	-0.34	2.16	2.50	2.50	2.5	[3]	<sup>2</sup>
CdS	sulfide	-0.46	1.94	2.40	2.00	2	[7]	
CdFe <sub>2</sub> O <sub>4</sub>	oxide	0.24	2.54	2.30	7.22	7.22	[7]	
<i>n</i> -Fe <sub>2</sub> O <sub>3</sub> (hematite)	oxide	0.34	2.54	2.20	8.60	8.6	[7, 5]	
CdO	oxide	0.17	2.37	2.20	11.60	11.6	[7]	
Cu <sub>2</sub> O	oxide	-0.22	1.98	2.20	8.53	8.53	[7]	
<i>n</i> -Ta <sub>3</sub> N <sub>5</sub>	nitride	-0.52	1.58	2.10	1.00	1	[3]	<sup>3</sup>
CuO	oxide	0.52	2.22	1.70	9.50	9.5	[7]	
<i>n</i> -CdSe	selenide	-1.00	0.70	1.70	12.00	NA	[4, 6]	
MoS <sub>2</sub>	sulfide	0.29	1.46	1.17	2.00	2	[7]	
PbS	sulfide	0.30	0.67	0.37	1.40	1.4	[7]	

<sup>1</sup> Band gap from diffuse reflectance spectroscopy, edges from Mott-Schottky.

<sup>2</sup> VB and CB from UPS measurement. Flatband potential expected to be a linear function of pH.

<sup>3</sup> VB and CB from UPS measurement. Flatband potential showed a Nernstian dependence on pH.

## xtable code chunk

```

xtab.semiconductors <-
  semiconductors %>%
  mutate(
    formula = ifelse(
      semiconductors$polymorph == "",
      paste0(
        ifelse(
          semiconductors$sctype == "",
          "",
          paste0("$", semiconductors$sctype, "$-")),
        "\\ch{" , semiconductors$formula, "}" ),
      paste0(
        ifelse(
          semiconductors$sctype == "",
          "",
          paste0("$", semiconductors$sctype, "$-")),
        "\\ch{" , semiconductors$formula, "}" , "(" , semiconductors$polymorph, ")" ) ) ) %>%
  mutate(
    pH = ifelse(
      is.na(semiconductors$pH),
      "\\multicolumn{1}{c}{\\texttt{NA}}",
      semiconductors$pH ) ) %>%
  mutate(
    pH.ZPC = ifelse(
      is.na(semiconductors$pH.ZPC),
      "\\multicolumn{1}{c}{\\texttt{NA}}",
      semiconductors$pH.ZPC ) ) %>%
  mutate(
    ref = ifelse(
      semiconductors$ref == "",
      "",
      paste0("\\cite{" , semiconductors$ref, "}") ) ) %>%
  mutate(
    footnotemark = ifelse(
      is.na(footnotemark),
      "",
      paste0("$~{" , footnotemark, "$") ) ) %>%
  select(formula, class, CB, VB, Eg, pH, pH.ZPC, ref, footnotemark) %>%
  xtable()
caption(xtab.semiconductors) <- paste(
  "Band edge levels at the pH of ZPC for each material.",
  "All band edge potentials vs SHE at the given pH for each semiconductor.",
  "The point of zero surface charge for each material is given (where available)",
  "in the column labelled $\\mathrm{pH}_{\\mathrm{ZPC}}$." )
label(xtab.semiconductors) <- "tab:semiconductors-asis"
names(xtab.semiconductors) <- c(
  "{Formula}",
  "{Class}",
  "{$E_{\\text{CB}}$/\\si{\\voltSHE}}",
  "{$E_{\\text{VB}}$/\\si{\\voltSHE}}",
  "{$E_{\\text{g}}$/\\si{\\volt}}",
  "{pH}",
  "{pH$_{\\text{ZPC}}$}",
  "{Ref}",
  "{Note}" )
digits(xtab.semiconductors) <- c(
  0, #row.names
  0, #formula
  0, #class
  2, #CB
  2, #VB
  2, #Eg
  2, #pH
  2, #pH.ZPC
  0, #Refs
  0) #Notes
display(xtab.semiconductors) <- c(
  "s", #row.names
  "s", #formula
  "s", #class
  "f", #CB
  "f", #VB
  "f", #Eg
  "f", #pH

```

```

"f", #pH.ZPC
"s", #Refs
"s") #Notes
align(xtab.semiconductors) <- c(
  "l", #row.names
  "l", #formula
  "l", #class
  "S[table-format=+1.2]", #CB
  "S[table-format=+1.2]", #VB
  "S[table-format=+1.2]", #Eg
  "S[table-format=2.2]", #pH
  "S[table-format=2.2]", #pH.ZPC
  "c", #Refs
  "l") #Notes
## create-latex-footnotetexts
footnotetext <- comments
# add numbering to each footnote
for (j in 1:length(comments)) {
  footnotetext[j] <- paste0(
    "\\multicolumn{" , dim(xtab.semiconductors)[2],
    "}{1}{", "$^{", j, "$ ", comments[j], "}",
    ifelse(
      j == length(comments),
      "\\n",
      "\\\\"))
}
print(
  xtab.semiconductors,
  floating = TRUE,
  floating.environment = "table",
  table.placement = "tbp",
  caption.placement = "top",
  hline.after = NULL,
  add.to.row = list(
    pos = list(
      -1,
      0,
      nrow(xtab.semiconductors),
      nrow(xtab.semiconductors)),
    command = c(
      "\\toprule\\n",
      "\\midrule\\n",
      "\\bottomrule\\n",
      paste(footnotetext, collapse = "\\n"))),
  include.rownames = FALSE,
  include.colnames = TRUE,
  type = "latex",
  tabular.environment = "tabular",
  latex.environments = c("center", "small"),
  # note: env small affects the table and footnotetext, but not the caption
  sanitize.text.function = function(x){x},
  math.style.negative = FALSE)

```

Source: data.Rnw  
git refs: (HEAD -> master)  
git hash: 11246a70f2abe6d2d671a5326d167ce37b6cfbb8  
git author: taha@luxor  
author email: taha@chepec.se  
commit date: 2018-03-12 14:21:31 +0100  
compile date: 2023-06-30 00:02:07

- R version 4.1.3 (2022-03-10), x86\_64-pc-linux-gnu
- Running under: Ubuntu 22.04.2 LTS
- Matrix products: default
- BLAS: /usr/lib/x86\_64-linux-gnu/blas/libblas.so.3.10.0
- LAPACK:  
/usr/lib/x86\_64-linux-gnu/lapack/liblapack.so.3.10.0
- Base packages: base, datasets, graphics, grDevices, methods, stats, utils
- Other packages: bandgaps 0.1.1.9000, common 0.0.2, dplyr 1.0.10, knitr 1.39, refelectrodes 0.0.0.9000, xtable 1.8-4
- Loaded via a namespace (and not attached): assertthat 0.2.1, cli 3.4.1, compiler 4.1.3, DBI 1.1.3, evaluate 0.15, fansi 1.0.3, filehash 2.4-3, generics 0.1.3, glue 1.6.2, grid 4.1.3, highr 0.9, lifecycle 1.0.3, magrittr 2.0.3, pillar 1.8.1, pkgconfig 2.0.3, R6 2.5.1, rlang 1.0.6, stringi 1.7.8, stringr 1.4.0, tibble 3.1.8, tidyselect 1.2.0, tikzDevice 0.12.3.1, tools 4.1.3, utf8 1.2.2, vctrs 0.5.1, withr 2.5.0, xfun 0.31

pdfTeX 3.141592653-2.6-1.40.25 (TeX Live 2023)  
kpathsea version 6.3.5  
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