Rendering all semiconductor `bandgaps` as a LaTeX table

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This package presents the position (potential) of the valence and conduction band edges for several 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 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, H^+ and OH^- are the dominant adsorbed species, and therefore the potential drop across the Helmholtz layer, V_H, and the flatband potential changes systematically with pH. The point of zero charge (PZP, also known as the potential of zero ζ potential, PZZP) is the pH at which the potential drop across the Helmoltz layer is zero. [5] The change of V_H with pH follows a straight-forward Nernstian relationship:

$$V_H/\mathrm{V} = 0.059\,\mathrm{V}(\mathrm{pH}_{PZC} - \mathrm{pH}) \tag{1}$$

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 variable `Nernstian` to the dataset which is set to 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 Ta2O5, TaON, and Ta3N5 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 CdSe and Coupled TiO2/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_{ZPC}.

Formula	Class	E_{CB}/V(SHE)	E_{VB}/V(SHE)	E_g/V	pH	pH_{ZPC}	Ref	Note
ZrO_2	oxide	−1.03	3.97	5.00	6.70	6.7	[7]	
Ta_2O_5	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_2	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]	
$KTaO_3$	oxide	−0.87	2.63	3.50	8.55	8.55	[7]	
$SrTiO_3$	oxide	−1.20	2.20	3.40	8.60	8.6	[7]	
$BaTiO_3$	oxide	0.14	3.44	3.30	9.00	9	[7]	
n-TiO_2 (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]	
n-TiO_2 (rutile)	oxide	−0.76	2.24	3.00	13.00	NA	[1]	
$CuTiO_3$	oxide	−0.12	2.87	2.99	7.29	7.29	[7]	
$FeTiO_3$	oxide	−0.15	2.65	2.80	6.30	6.3	[7]	
SiC	carbide	−0.46	2.34	2.80	14.00	NA	[2]	1
In_2O_3	oxide	−0.56	2.24	2.80	8.64	8.64	[7]	
WO_3	oxide	0.80	3.50	2.70	0.43	0.43	[7]	
n-TaON	oxynitride	−0.34	2.16	2.50	2.50	2.5	[3]	2
CdS	sulfide	−0.46	1.94	2.40	2.00	2	[7]	
$CdFe_2O_4$	oxide	0.24	2.54	2.30	7.22	7.22	[7]	
n-Fe_2O_3 (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_2O	oxide	−0.22	1.98	2.20	8.53	8.53	[7]	
n-Ta_3N_5	nitride	−0.52	1.58	2.10	1.00	1	[3]	3
CuO	oxide	0.52	2.22	1.70	9.50	9.5	[7]	
n-CdSe	selenide	−1.00	0.70	1.70	12.00	NA	[4, 6]	
MoS_2	sulfide	0.29	1.46	1.17	2.00	2	[7]	
PbS	sulfide	0.30	0.67	0.37	1.40	1.4	[7]	

[1] Band gap from diffuse reflectance spectroscopy, edges from Mott-Schottky.
[2] VB and CB from UPS measurement. Flatband potential expected to be a linear function of pH.
[3] 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 $\\mathrm{pH_{ZPC}}$.")
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=1.2]",  #pH
   "S[table-format=1.2]",  #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],
             "}{l}{", "$^{", j, "}$ ", 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: 2019-10-17 06:11:32

```
## Untracked files:
##  Untracked:  R/baseplot.R
##  Untracked:  README.md
##  Untracked:  inst/
##  Untracked:  man/plot_bandgaps.Rd
##  Untracked:  vignettes/.build.timestamp
##  Untracked:  vignettes/diagram.Rnw
##
## Unstaged changes:
##  Modified:   .Rbuildignore
##  Modified:   .gitignore
##  Modified:   DESCRIPTION
##  Modified:   NAMESPACE
##  Modified:   R/data.R
##  Modified:   R/functions.R
##  Modified:   bandgaps.Rproj
##  Deleted:    data-raw/semiconductors.R
##  Modified:   data/semiconductors.rda
##  Modified:   man/semiconductor_row.Rd
##  Modified:   man/semiconductors.Rd
##  Modified:   vignettes/data.R
##  Modified:   vignettes/data.Rnw
##  Deleted:    vignettes/data.pdf
##  Modified:   vignettes/references.bib
```

- R version 3.6.1 (2019-07-05), x86_64-pc-linux-gnu
- Running under: Ubuntu 16.04.6 LTS
- Matrix products: default
- BLAS: /usr/lib/libblas/libblas.so.3.6.0
- LAPACK: /usr/lib/lapack/liblapack.so.3.6.0
- Base packages: base, datasets, graphics, grDevices, methods, stats, utils
- Other packages: bandgaps 0.0.0.9003, common 0.0.1.9000, dplyr 0.8.3, git2r 0.26.1, here 0.1, knitr 1.25, refelectrodes 0.0.0.9000, xtable 1.8-4
- Loaded via a namespace (and not attached): assertthat 0.2.1, backports 1.1.5, callr 3.3.2, cli 1.1.0, compiler 3.6.1, crayon 1.3.4, curl 4.2, desc 1.2.0, devtools 2.2.1, digest 0.6.21, ellipsis 0.3.0, evaluate 0.14, filehash 2.4-2, fs 1.3.1, glue 1.3.1, grid 3.6.1, highr 0.8, magrittr 1.5, memoise 1.1.0, pillar 1.4.2, pkgbuild 1.0.6, pkgconfig 2.0.3, pkgload 1.0.2, prettyunits 1.0.2, processx 3.4.1, ps 1.3.0, purrr 0.3.2, R6 2.4.0, Rcpp 1.0.2, remotes 2.1.0, rlang 0.4.0, rprojroot 1.3-2, rstudioapi 0.10, sessioninfo 1.1.1, stringi 1.4.3, stringr 1.4.0, testthat 2.2.1, tibble 2.1.3, tidyselect 0.2.5, tikzDevice 0.12.3, tools 3.6.1, usethis 1.5.1, withr 2.1.2, xfun 0.10

```
pdfTeX 3.14159265-2.6-1.40.19 (TeX Live 2018)
kpathsea version 6.3.0
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Primary author of pdfTeX: Han The Thanh (pdfTeX) et al.
Compiled with libpng 1.6.34; using libpng 1.6.34
Compiled with zlib 1.2.11; using zlib 1.2.11
Compiled with xpdf version 4.00
```