Rendering all semiconductor `bandgaps` as a LaTeX table

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Here we display the data in `bandgaps::semiconductors` as a table (see table 1). To make the rendered table look nice, we will compress some columns and put any comments into tabular footnotes, but we will include all the data in the `bandgaps` dataset.
We will render the table using `xtable` (that chunk is shown at the end of this document).

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 cadmium selenide and coupled titania/cadmium selenide 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.

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]	[2]
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.

`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.")
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: 2018-03-16 04:36:37

```
## Unstaged changes:
##  Modified:   DESCRIPTION
##  Modified:   vignettes/data.R
##  Modified:   vignettes/data.Rnw
##  Deleted:    vignettes/data.pdf
##  Modified:   vignettes/references.bib
```

- R version 3.4.3 (2017-11-30), `x86_64-pc-linux-gnu`
- Running under: `Ubuntu 16.04.3 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, grDevices, graphics, methods, stats, utils
- Other packages: bandgaps 0.0.0.9002, bindrcpp 0.2, common 0.0.0.9009, dplyr 0.7.4, ggplot2 2.2.1, git2r 0.21.0, knitr 1.20, magrittr 1.5, xtable 1.8-2
- Loaded via a namespace (and not attached): R6 2.2.2, Rcpp 0.12.15, assertthat 0.2.0, backports 1.1.2, bindr 0.1, colorspace 1.3-2, commonmark 1.4, compiler 3.4.3, crayon 1.3.4, desc 1.1.1, devtools 1.13.5, digest 0.6.15, evaluate 0.10.1, filehash 2.4-1, glue 1.2.0, grid 3.4.3, gtable 0.2.0, highr 0.6, lazyeval 0.2.1, memoise 1.1.0, munsell 0.4.3, pillar 1.2.1, pkgconfig 2.0.1, plyr 1.8.4, rlang 0.2.0, roxygen2 6.0.1, rprojroot 1.3-2, rstudioapi 0.7, scales 0.5.0, stringi 1.1.6, stringr 1.3.0, tibble 1.4.2, tikzDevice 0.10-1.2, tools 3.4.3, withr 2.1.1, xml2 1.2.0

```
pdfTeX 3.14159265-2.6-1.40.18 (TeX Live 2017)
kpathsea version 6.2.3
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Compiled with zlib 1.2.11; using zlib 1.2.11
Compiled with xpdf version 3.04
```