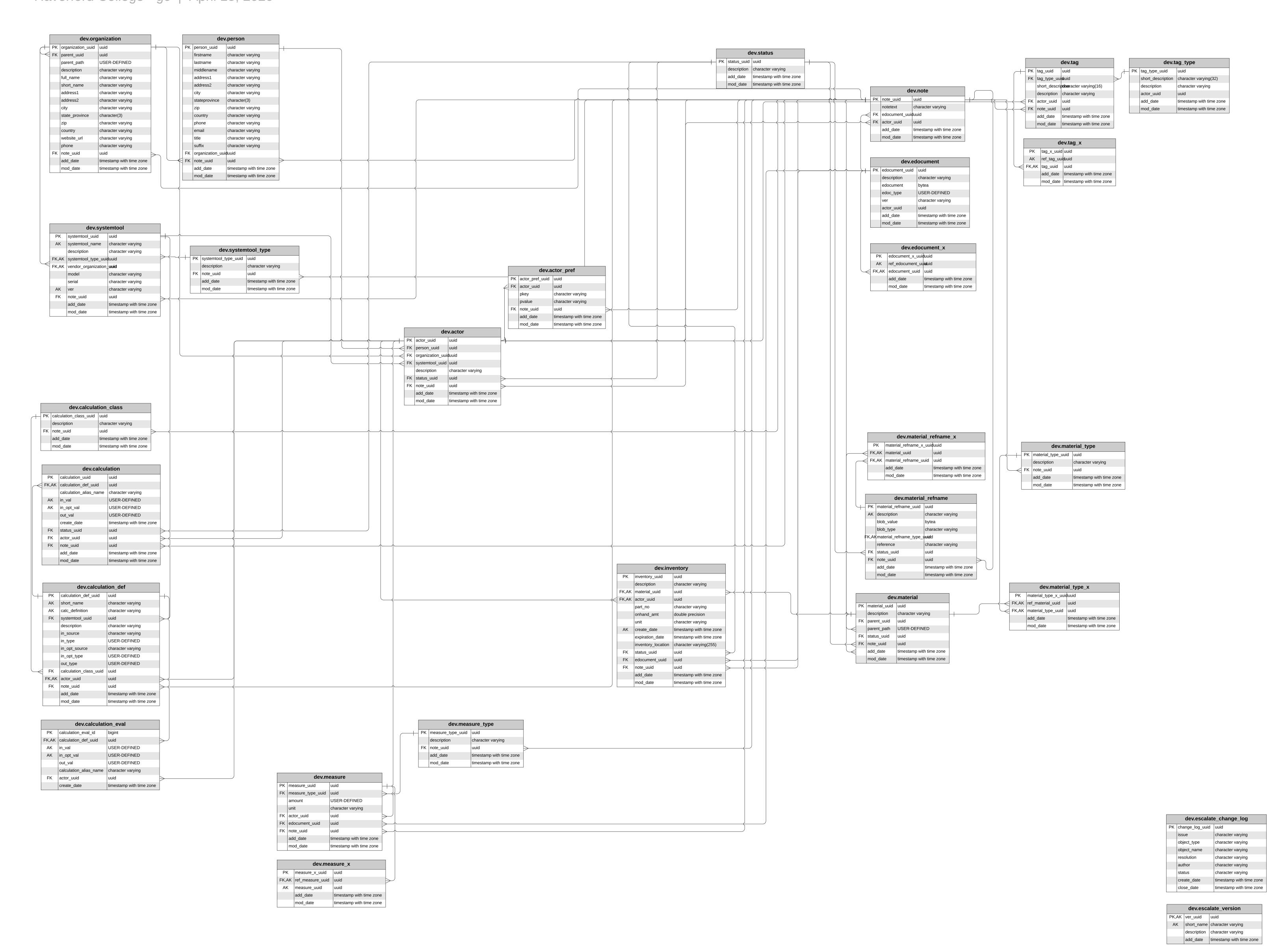
## **ESCALATE v3 Data Model**

Haverford College - gc | April 15, 2020



amount

character varying(255) update\_date | timestamp with time zone create\_date | timestamp with time zone updated\_by character varying(255) in\_stock real remaining\_stockal

character varying(255) double precision character varying(255) update\_date | timestamp with time zone create\_date | timestamp with time zone

dev.load perov desc def

short\_name character varying(255) calc\_definition | character varying(255) description character varying(255) systemtool\_nameharacter varying(255) systemtool\_ver | character varying(255) in\_calc\_source | character varying(255) in\_type character varying(255) in\_opt\_calc\_soundearacter varying(255) in\_opt\_type character varying(255) out\_type character varying(255)

dev.load\_perov\_mol\_image filename character varying mol\_name character varying

dev.load hc inventory character varying(255) double precision

dev.load\_lbl\_inventory

character varying(255)

\_image bytea

smallint \_feat\_heteroaliphaticringcount \_feat\_heteroaromaticringcount \_feat\_rotatablebondcount \_feat\_balabanindex double precision smallint \_feat\_cyclomaticnumber smallint \_feat\_hyperwienerindex \_feat\_wienerindex smallint \_feat\_wienerpolarity double precision \_feat\_minimalprojectionarea \_feat\_maximalprojectionarea double precision double precision \_feat\_minimalprojectionradius \_feat\_maximalprojectionradius double precision \_feat\_lengthperpendiculartotheminarea | double precision \_feat\_lengthperpendiculartothemaxarea | double precision \_feat\_vanderwaalsvolume double precision feat vanderwaalssurfacearea double precision \_feat\_asa double precision \_feat\_asa+ double precision \_feat\_asadouble precision \_feat\_asa\_h double precision \_feat\_asa\_p double precision \_feat\_polarsurfacearea double precision \_feat\_acceptorcount smallint \_feat\_accsitecount \_feat\_donorcount \_feat\_fr\_nh2 smallint \_feat\_fr\_nh1 \_feat\_fr\_nh0 \_feat\_fr\_quatn smallint smallint \_feat\_fr\_arn \_feat\_fr\_ar\_nh smallint \_feat\_fr\_imine \_feat\_fr\_amidine \_feat\_fr\_dihydropyridine \_feat\_fr\_guanido \_feat\_fr\_piperdine smallint \_feat\_fr\_piperzine \_feat\_fr\_pyridine \_feat\_maximalprojectionsize double precision double precision \_feat\_minimalprojectionsize \_feat\_molsurfaceareavdwp double precision \_feat\_msareavdwp double precision \_feat\_molsurfaceareaasap double precision \_feat\_msareaasap double precision \_feat\_protpolarsurfacearea double precision \_feat\_protpsa double precision \_feat\_hacceptorcount \_feat\_hdonorcount \_feat\_charge\_cnt double precision \_calc\_chrg\_per\_vol \_calc\_chrg\_per\_asa double precision

dev.load\_perov\_desc

\_raw\_smiles

\_raw\_molweight

\_raw\_smiles\_standard

\_raw\_standard\_molweight

\_prototype\_ecpf4\_256\_6

\_feat\_atomcount\_c

\_feat\_atomcount\_n

\_feat\_avgpol

\_feat\_molpol

\_feat\_refractivity

\_feat\_bondcount

\_feat\_aliphaticringcount

\_feat\_aromaticringcount

\_feat\_aliphaticatomcount

\_feat\_aromaticatomcount

\_feat\_carboaliphaticringcount

\_feat\_carboaromaticringcount

\_feat\_carboringcount

feat chainatomcount

\_feat\_chiralcentercount

\_feat\_ringatomcount

\_feat\_smallestringsize

\_feat\_largestringsize

character varying(255)

character varying(255)

double precision

double precision

double precision

character varying

double precision

double precision

double precision

smallint

smallint

smallint

smallint

smallint

smallint

smallint

character varying(255